CRYSTAL STRUCUTRE OF KETOPANTOATE HYDROXYMETHYLTRANSFERASE

eld of the Invention

The present invention relates to the enzyme ketopantoate hydroxymethyltransferase (KPHMT), and in particular its crystal structure and the use of this structure in drug discovery.

Background of the Invention

Pantothenic acid (vitamin B_5) is found in coenzyme A (CoA) and the acyl carrier protein (ACP), both of which are involved in fatty acid metabolism.

Pantothenic acid can be synthesised by plants and microorganisms but animals are apparently unable to make the vitamin, and require it in their diet. However, all organisms are able to convert pantothenic acid to its metabolically active form, coenzyme A.

The pathway for the synthesis of pantothenic acid is shown in Figure 1. It provides a potential target for the treatment of infectious disease, since inhibitors of the pathway should be damaging to bacteria and fungi but not to human or animal subjects infected by such microorganisms.

Of specific interest is ketopantoate hydroxymethyltransferase (KPHMT (SEQ ID NOs: 7-11, for example); 5,10-methylenetetrahydrofolate: α -ketoisovalerate hydroxymethyl transferase, EC 2.1.2.11). Powers et al. (1) showed that KPHMT (SEQ ID NOs: 7-11, for example) is a class II aldolase that utilizes 5,10-CH₂-H₄folate (mTHF) to transfer a hydroxymethyl group to α -ketoisovalerate (α -KIVA) and thereby form ketopantoate, as shown in Figure 2. This is the first step in pantothenic acid biosynthesis. Inhibitors (whether competitive, non-competitive, uncompetitive or irreversible) of KPHMT (SEQ ID NOs: 7-11, for example) would be of significant technical and commercial interest.

KPHMT (SEQ ID NOs: 7-11, for example) from Escherichia coli has been cloned and over-expressed in E. coli., and was the

first sequence of a pantothenate enzyme to be determined (2). The recombinant protein has 264 amino acids, corresponding to a molecular weight of 28,237 Da. The oligomeric state of the enzyme appears to be organism specific. The homologue from the lower eukaryote, Aspergillus nidulans, has been expressed in an active form in E. coli and shown to be an octamer by gel filtration chromatography (3). However, the E. coli enzyme, was found to be a decamer by sedimentation equilibrium experiments, gel filtration chromatography and polyacrylamide gel electrophoresis under native conditions (1).

Very little is known about the mode of action of KPHMT (SEQ ID NOs: 7-11, for example), except that the addition of the hydroxymethyl group proceeds with retention of configuration (4). Mg²⁺ is essential for activity, whilst metal reconstitution experiments with Mn²⁺, Co²⁺ and Zn²⁺ give enzyme with progressively less activity (1). To date, five ketopantoate auxotrophs, from E. coli., A. nidulans, Daturia innoxia and two from Salmonella typhymurium, have been identified (5)(6). Four of these (from E. coli, A. nidulans, and the two from Salmonella typhymurium) have been shown to have defects in the panB gene which encodes KPHMT (SEQ ID NOs: 7-11, for example). The fifth (from the plant, D. innoxia) is suspected to have a panB defect (6). The A. nidulans auxotroph is caused by a deletion of Gly 168 (corresponding to Gly 205 in E. coli).

Until now no one has successfully determined the structure of KPHMT (SEQ ID NOs: 7-11, for example). This has prevented KPHMT (SEQ ID NOs: 7-11, for example) inhibitors being developed via structure-based drug design methodologies. Therefore, knowledge of the structure of KPHMT (SEQ ID NOs: 7-11, for example) would significantly assist the rational design of novel therapeutics based on KPHMT (SEQ ID NOs: 7-11, for example) inhibitors.

Definitions

In the following by "binding site" we mean a site (such as an atom, a functional group of an amino acid residue or a plurality of such atoms and/or groups) in a KPHMT (SEQ ID NOs: 7-11, for example) binding cavity which may bind to an agent compound such as a candidate inhibitor. Depending on the particular molecule in the cavity, sites may exhibit attractive or repulsive binding interactions, brought about by charge, steric considerations and the like.

By "fitting", is meant determining by automatic, or semi-automatic means, interactions between one or more atoms of an agent molecule and one or more atoms or binding sites of the KPHMT (SEQ ID NOs: 7-11, for example), and calculating the extent to which such interactions are stable. Various computer-based methods for fitting are described further herein.

By "root mean square deviation" we mean the square root of the arithmetic mean of the squares of the deviations from the mean.

By a "computer system" we mean the hardware means, software means and data storage means used to analyse atomic coordinate data. The minimum hardware means of the computer-based systems of the present invention comprises a central processing unit (CPU), input means, output means and data storage means. Desirably a monitor is provided to visualise structure data. The data storage means may be RAM or means for accessing computer readable media of the invention. Examples of such systems are microcomputer workstations available from Silicon Graphics Incorporated and Sun Microsystems running Unix based, Windows NT or IBM OS/2 operating systems.

By "computer readable media" we mean any media which can be read and accessed directly by a computer e.g. so that the media is suitable for use in the above-mentioned computer system. Such media include, but are not limited to: magnetic storage media such as floppy discs, hard disc storage medium and magnetic tape; optical storage media such as optical discs or

CD-ROM; electrical storage media such as RAM and ROM; and hybrids of these categories such as magnetic/optical storage media.

Summary of the Invention

The present invention is at least partly based on overcoming several technical hurdles: we have (i) produced KPHMT (SEQ ID NOS: 7-11, for example) crystals of suitable quality, including crystals of selenium atom KPHMT (SEQ ID NOS: 7-11, for example) derivatives, for performing X-ray diffraction analyses, (ii) collected X-ray diffraction data from the crystals, (iii) determined the three-dimensional structure of KPHMT (SEQ ID NOS: 7-11, for example), and (iv) identified binding sites on the enzyme which are likely to be involved in the enzymatic reaction.

In general aspects, the present invention is concerned with identifying or obtaining agent compounds (especially inhibitors of KPHMT (SEQ ID NOs: 7-11, for example)) for modulating KPHMT (SEQ ID NOs: 7-11, for example) activity, and in preferred embodiments identifying or obtaining actual agent compounds/inhibitors. Crystal structure information presented herein is useful in designing potential inhibitors and modelling them or their potential interaction with the KPHMT (SEQ ID NOs: 7-11, for example) binding cavity. Potential inhibitors may be brought into contact with KPHMT (SEQ ID NOs: 7-11, for example) to test for ability to interact with the KPHMT (SEQ ID NOs: 7-11, for example) binding cavity. Actual inhibitors may be identified from among potential inhibitors synthesized following design and model work performed in silico. An inhibitor identified using the present invention may be formulated into a composition, for instance a composition comprising a pharmaceutically acceptable excipient, and may be used in the manufacture of a medicament for use in a method of treatment. These and other aspects and embodiments of the present invention are discussed below.

In a first aspect, the present invention provides a crystal of KPHMT (SEQ ID NOs: 7-11, for example) having a monoclinic space group $P2_1$, and unit cell dimensions of a = 86.1 Å, b = 157.2 Å, c = 100.2 Å and β = 97.4°, or more generally a = 86.1±0.2 Å, b = 157.2±0.2 Å, c = 100.2±0.2 Å and β = 97.4±0.2°.

We have found that the asymmetric unit of such a crystal corresponds to a KPHMT (SEQ ID NOs: 7-11, for example) decamer which may be thought of as a pentamer of KPHMT (SEQ ID NOs: 7-11, for example) dimers, the dimers being related by a non-crystallographic five-fold axis

Alternatively, or additionally, the crystal may have the three dimensional atomic coordinates of Table 1. An advantageous feature of the structural data according to Table 1 are that they have a high resolution of about 1.8 Å.

The coordinates of Table 1 provide a measure of atomic location in Angstroms, to a first decimal place. The coordinates are a relative set of positions that define a shape in three dimensions, so it is possible that an entirely different set of coordinates having a different origin and/or axes could define a similar or identical shape. Furthermore, varying the relative atomic positions of the atoms of the structure so that the root mean square deviation of the residue backbone atoms (i.e. the nitrogen-carbon-carbon backbone atoms of the protein amino acid residues) is less than 1.5 Å (preferably less than 1.0 Å and more preferably less than 0.5 Å) when superimposed on the coordinates provided in Table 1 for the residue backbone atoms, will generally result in a structure which is substantially the same as the structure of Table 1 in terms of both its structural characteristics and potency for structure-based design of KPHMT (SEQ ID NOs: 7-11, for example) inhibitors. Likewise changing the number and/or positions of the water molecules and/or substrate molecules of Table 1 will not generally affect the potency of the structure for structure-based design of KPHMT (SEQ ID NOs: 7-11, for example) inhibitors. Thus for the purposes described herein as being aspects of the present

invention, it is within the scope of the invention if: the Table 1 coordinates are transposed to a different origin and/or axes; the relative atomic positions of the atoms of the structure are varied so that the root mean square deviation of residue backbone atoms is less than 1.5 Å (preferably less than 1.0 Å and more preferably less than 0.5 Å) when superimposed on the coordinates provided in Table 1 for the residue backbone atoms; and/or the number and/or positions of water molecules and/or substrate molecules is varied. Reference herein to the coordinate data of Table 1 thus includes the coordinate data in which one or more individual values of the Table are varied in this way.

Also, modifications in the KPHMT (SEQ ID NOs: 7-11, for example) crystal structure due to e.g. mutations, additions, substitutions, and/or deletions of amino acid residues (including the deletion of one or more KPHMT (SEQ ID NOs: 7-11, for example) protomers) could account for variations in the KPHMT (SEQ ID NOs: 7-11, for example) atomic coordinates. However, atomic coordinate data of KPHMT (SEQ ID NOs: 7-11, for example) modified so that a ligand that bound to one or more binding sites of KPHMT (SEQ ID NOs: 7-11, for example) would be expected to bind to the corresponding binding sites of the modified KPHMT (SEQ ID NOs: 7-11, for example) are, for the purposes described herein as being aspects of the present invention, also within the scope of the invention. Reference herein to the coordinates of Table 1 thus includes the coordinates modified in this way. Preferably, the modified coordinate data define at least one KPHMT (SEQ ID NOs: 7-11, for example) binding cavity.

In a further aspect, the invention provides a method for crystallizing a selenomethionine KPHMT (SEQ ID NOs: 7-11, for example) derivative which comprises producing KPHMT (SEQ ID NOs: 7-11, for example) by recombinant production in a bacterial host (e.g. E. coli) in the presence of selenomethionine, recovering a selenomethionine KPHMT (SEQ ID NOs: 7-11, for example)

derivative from the host and growing crystals from the recovered selenomethionine KPHMT (SEQ ID NOs: 7-11, for example) derivative.

Thus, the selenium atom KPHMT (SEQ ID NOs: 7-11, for example) derivative and KPHMT (SEQ ID NOs: 7-11, for example) produced by crystallising native KPHMT (SEQ ID NOs: 7-11, for example) (see the detailed description below) are provided as crystallised proteins suitable for X-ray diffraction analysis.

The crystals may be grown by any suitable method, e.g. the hanging drop method.

In another aspect, the invention provides a method of analysing a KPHMT (SEQ ID NOs: 7-11, for example)—ligand complex comprising the step of employing (i) X-ray crystallographic diffraction data from the KPHMT (SEQ ID NOs: 7-11, for example)—ligand complex and (ii) a three-dimensional structure of KPHMT (SEQ ID NOs: 7-11, for example) to generate a difference Fourier electron density map of the complex, the three-dimensional structure being defined by atomic coordinate data according to Table 1.

Therefore, KPHMT (SEQ ID NOs: 7-11, for example)—ligand complexes can be crystallised and analysed using X-ray diffraction methods, e.g. according to the approach described by Greer et al., J. of Medicinal Chemistry, Vol. 37, (1994), 1035—1054, and difference Fourier electron density maps can be calculated based on X-ray diffraction patterns of soaked or co-crystallised KPHMT (SEQ ID NOs: 7-11, for example) and the solved structure of un-complexed KPHMT (SEQ ID NOs: 7-11, for example). These maps can then be used to determine whether and where a particular ligand binds to KPHMT (SEQ ID NOs: 7-11, for example) and/or changes the conformation of KPHMT (SEQ ID NOs: 7-11, for example).

Electron density maps can be calculated using programs such as those from the CCP4 computing package (Collaborative Computational Project 4. The CCP4 Suite: Programs for Protein Crystallography, Acta Crystallographica, D50, (1994), 760-763.).

For map visualisation and model building programs such as O (Jones et al., *Acta Crystallograhy*, A47, (1991), 110-119) can be used.

In another aspect, the present invention provides a method for identifying an agent compound (e.g. an inhibitor) which modulates KPHMT (SEQ ID NOs: 7-11, for example) activity, comprising the steps of:

- (a) employing three-dimensional atomic coordinate data according to Table 1 to characterise at least a plurality of KPHMT (SEQ ID NOs: 7-11, for example) binding sites;
 - (b) providing the structure of a candidate agent compound;
- (c) fitting the candidate agent compound to the binding sites; and
 - (d) selecting the candidate agent compound.

Preferably sufficient binding sites are characterised to define a KPHMT (SEQ ID NOs: 7-11, for example) binding cavity.

A plurality (for example two, three or four) of spaced KPHMT (SEQ ID NOs: 7-11, for example) binding sites may be characterised and a plurality of respective compounds designed or selected. The agent compound may then be formed by linking the respective compounds into a larger compound which maintains the relative positions and orientations of the respective compounds at the binding sites. The larger compound may be formed as a real molecule or by computer modelling.

In any event, the determination of the three-dimensional structure of KPHMT (SEQ ID NOs: 7-11, for example) provides a basis for the identification of new and specific ligands for KPHMT (SEQ ID NOs: 7-11, for example) e.g. by computer modelling.

More specifically, a potential modulator of KPHMT (SEQ ID NOs: 7-11, for example) activity can be examined through the use of computer modelling using a docking program such as GRAM, DOCK, or AUTODOCK (see Walters et al., Drug Discovery Today, Vol.3, No.4, (1998), 160-178, and Dunbrack et al., Folding and Design, 2, (1997), 27-42). This procedure can include computer

fitting of candidate inhibitors to KPHMT (SEQ ID NOs: 7-11, for example) to ascertain how well the shape and the chemical structure of the candidate inhibitor will bind to the enzyme.

Also computer-assisted, manual examination of the binding cavity structure of KPHMT (SEQ ID NOs: 7-11, for example) may be performed. The use of programs such as GRID (Goodford, *J. Med. Chem.*, 28, (1985), 849-857) - a program that determines probable interaction sites between molecules with various functional groups and the enzyme surface - may also be used to analyse the binding cavity to predict partial structures of inhibiting compounds.

Computer programs can be employed to estimate the attraction, repulsion, and steric hindrance of the two binding partners (e.g. the KPHMT (SEQ ID NOs: 7-11, for example) and a candidate inhibitor). Generally the tighter the fit, the fewer the steric hindrances, and the greater the attractive forces, the more potent the potential modulator since these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a potential drug, the more likely it is that the drug will not interact with other proteins as well. This will tend to minimise potential side-effects due to unwanted interactions with other proteins.

In one embodiment a plurality of candidate agent compounds are screened or interrogated for interaction with the binding sites. In one example, step (b) involves providing the structures of the candidate agent compounds, each of which is then fitted in step (c) to computationally screen a database of compounds (such as the Cambridge Structural Database) for interaction with the binding sites. In another example, a 3-D descriptor for the agent compound is derived, the descriptor including e.g. geometric and functional constraints derived from the architecture and chemical nature of the binding cavity. The descriptor may then be used to interrogate the compound database, the identified agent compound being the compound which

matches with the features of the descriptor. In effect, the descriptor is a type of virtual pharmacophore.

Having designed or selected possible binding partners, these can then be screened for activity. Consequently, the method preferably comprises the further steps of:

- (e) obtaining or synthesising the candidate agent compound; and
- (f) contacting the candidate agent compound with KPHMT (SEQ ID NOs: 7-11, for example) to determine the ability of the candidate agent compound to interact with KPHMT (SEQ ID NOs: 7-11, for example).

In step (e) the candidate agent compound may be contacted with KPHMT (SEQ ID NOs: 7-11, for example) in the presence of a substrate, and typically a buffer, to determine the ability of the candidate agent compound to inhibit KPHMT (SEQ ID NOs: 7-11, for example). The substrate may be e.g., one or both of 5,10- $\mathrm{CH_2}\text{-H_4}\mathrm{folate}$, α -ketoisovalerate, or salts thereof. So, for example, an assay mixture for KPHMT (SEQ ID NOs: 7-11, for example) may be produced which comprises the candidate inhibitor, substrate and buffer.

Instead of, or in addition to, performing e.g. a chemical assay, the method may comprise the further steps of:

- (e) obtaining or synthesising the candidate agent compound;
- (f) forming a complex of KPHMT (SEQ ID NOs: 7-11, for example) and the candidate agent compound; and
- (g) analysing (e.g. by the method of an earlier aspect of the invention) said complex by X-ray crystallography or NMR spectroscopy to determine the ability of the candidate agent compound to interact with KPHMT (SEQ ID NOs: 7-11, for example).

Detailed structural information can then be obtained about the binding of the agent compound to KPHMT (SEQ ID NOs: 7-11, for example), and in the light of this information adjustments can be made to the structure or functionality of the compound, e.g. to improve binding to the binding cavity. Steps (e) to (g) may be repeated and re-repeated as necessary. For X-ray

crystallographic analysis, the complex may be formed by crystal soaking or co-crystallisation.

In another aspect, the invention includes a compound which is identified as a modulator of KPHMT (SEQ ID NOs: 7-11, for example) activity by the method of the fourth aspect.

Following identification of an inhibitor compound, it may be manufactured and/or used in the preparation, i.e. manufacture or formulation, of a composition such as a medicament, pharmaceutical composition or drug. These may be administered to individuals.

Thus, the present invention extends in various aspects not only to an inhibitor as provided by the invention, but also a pharmaceutical composition, medicament, drug or other composition comprising such an inhibitor e.g. for treatment (which may include preventative treatment) of disease such as microbial infection; a method comprising administration of such a composition to a patient, e.g. for treatment of disease such as microbial infection; use of such an inhibitor in the manufacture of a composition for administration, e.g. for treatment of disease such as microbial infection; and a method of making a pharmaceutical composition comprising admixing such an inhibitor with a pharmaceutically acceptable excipient, vehicle or carrier, and optionally other ingredients.

In another aspect, the invention relates to a method of determining three dimensional structures of KPHMT (SEQ ID NOs: 7-11, for example) homologues of unknown structure by utilising the structural coordinates of Table 1.

For example, if X-ray crystallographic or NMR spectroscopic data is provided for a KPHMT (SEQ ID NOs: 7-11, for example) homologue of unknown structure, the structure of KPHMT (SEQ ID NOs: 7-11, for example) as defined by Table 1 may be used to interpret that data to provide a likely structure for the KPHMT (SEQ ID NOs: 7-11, for example) homologue by techniques which are well known in the art, e.g. phase modelling in the case of X-ray crystallography.

One embodiment of the method comprises the steps of:

- (a) aligning a representation of an amino acid sequence of a KPHMT (SEQ ID NOs: 7-11, for example) homologue of unknown structure with the amino acid sequence of KPHMT (SEQ ID NOs: 7-11, for example) to match homologous regions of the amino acid sequences;
- (b) modelling the structure of the matched homologous regions of the KPHMT (SEQ ID NOs: 7-11, for example) of unknown structure on the structure as defined by Table 1 of the corresponding regions of KPHMT (SEQ ID NOs: 7-11, for example); and
- (c) determining a conformation (e.g. so that favourable interactions are formed within the KPHMT (SEQ ID NOs: 7-11, for example) of unknown structure and/or so that a low energy conformation is formed) for the KPHMT (SEQ ID NOs: 7-11, for example) of unknown structure which substantially preserves the structure of said matched homologous regions.

The term "homologous regions" describes amino acid residues in two sequences that are identical or have similar (e.g. aliphatic, aromatic, polar, negatively charged, or positively charged) side-chain chemical groups. Identical and similar residues in homologous regions are sometimes described as being respectively "invariant" and "conserved" by those skilled in the art.

Preferably one or all of steps (a) to (c) are performed by computer modelling.

Homology modelling is a technique that is well known to those skilled in the art (see e.g. Greer, *Science*, Vol. 228, (1985), 1055, and Blundell et al., Eur. J. Biochem, Vol. 172, (1988), 513).

In general, comparison of amino acid sequences is accomplished by aligning the amino acid sequence of a polypeptide of a known structure with the amino acid sequence of the polypeptide of unknown structure. Amino acids in the sequences are then compared and groups of amino acids that are

homologous are grouped together. This method detects conserved regions of the polypeptides and accounts for amino acid insertions or deletions.

Homology between amino acid sequences can be determined using commercially available algorithms. The programs *BLAST*, gapped BLAST, BLASTN and PSI-BLAST (provided by the National Center for Biotechnology Information) are widely used in the art for this purpose, and can align homologous regions of two amino acid sequences.

Once the amino acid sequences of the polypeptides with known and unknown structures are aligned, the structures of the conserved amino acids in a computer representation of the polypeptide with known structure are transferred to the corresponding amino acids of the polypeptide whose structure is unknown. For example, a tyrosine in the amino acid sequence of known structure may be replaced by a phenylalanine, the corresponding homologous amino acid in the amino acid sequence of unknown structure.

The structures of amino acids located in non-conserved regions may be assigned manually by using standard peptide geometries or by molecular simulation techniques, such as molecular dynamics (7). The final step in the process is accomplished by refining the entire structure using molecular dynamics and/or energy minimization.

In another aspect, the present invention provides systems, particularly a computer systems, intended to generate structures and/or perform rational drug design for KPHMT (SEQ ID NOS: 7-11, for example) - ligand complexes or KPHMT (SEQ ID NOS: 7-11, for example) homologues, the systems containing either (a) atomic coordinate data according to Table 1, said data defining the three-dimensional structure of KPHMT (SEQ ID NOS: 7-11, for example), or (b) structure factor data for KPHMT (SEQ ID NOS: 7-11, for example), said structure factor data being derivable from the atomic coordinate data of Table 1.

In another aspect, the present invention provides computer readable media with either (a) atomic coordinate data according to Table 1 recorded thereon, said data defining the three-dimensional structure of KPHMT (SEQ ID NOs: 7-11, for example), or (b) structure factor data for KPHMT (SEQ ID NOs: 7-11, for example) recorded thereon, the structure factor data being derivable from the atomic coordinate data of Table 1.

By providing such computer readable media, the atomic coordinate data can be routinely accessed to model KPHMT (SEQ ID NOS: 7-11, for example). For example, RASMOL (Sayle et al., TIBS, Vol. 20, (1995), 374) is a publicly available computer software package which allows access and analysis of atomic coordinate data for structure determination and/or rational drug design.

On the other hand, structure factor data, which are derivable from atomic coordinate data (see e.g. Blundell et al., in Protein Crystallography, Academic Press, New York, London and San Francisco, (1976)), are particularly useful for calculating e.g. difference Fourier electron density maps.

Brief Description of the Drawings

Figure 1 shows the pathway for the synthesis of pantothenic acid;

Figure 2 shows the chemical reaction between $\alpha\text{-KIVA}$ and $5,10\text{-CH}_2\text{-H}_4\text{folate}$ which is catalysed by KPHMT (SEQ ID NOs: 7-11, for example);

Figures 3a and b show ribbon representations of the decameric structure as viewed respectively along and from the side of the non-crystallographic five-fold axis;

Figures 4a and b show ribbon representations of respectively top and side views of a protomer;

Figure 5 shows a sequence alignment between primary structure among five members of the KPHMT (SEQ ID NOs: 7-11, for example) family and the secondary structure of the E. coli enzyme (SEQ ID NOs: 7-12, respectively);

Figure 6 shows a stereo pair wire-frame electron density map of the substrate binding site with a ketopantoate product molecule (KPL) and a metal ion believed to be Mg²⁺ on which the enzyme is dependent for its activity;

Figure 7 shows an electrostatic potential map for a protomer viewed looking towards the opening mouth of the binding cavity;

Figure 8 shows a stereo pair ribbon representation of the KPHMT (SEQ ID NOs: 7-11, for example) binding cavity;

Figure 9 shows a schematic representation of the distorted octahedral binding site for Mg^{2+} in the KPHMT (SEQ ID NOs: 7-11, for example) binding cavity;

Figures 10 and b show respectively side and top view stereo pair ribbon representations of the mouth of the KPHMT (SEQ ID NOS: 7-11, FOR EXAMPLE) binding cavity; and

Figures 11a and b show stereo pair ribbon representations of respectively (a) the binding cavities of a KPHMT (SEQ ID NOs: 7-11, for example) dimer, and (b) the interface between adjacent KPHMT dimers.

Detailed Description of the Invention

The present invention is founded on the determination of the three dimensional atomic structure of KPHMT (SEQ ID NOs: 7-11, for example).

Solving the Crystal Structure

1. Preparation of Recombinant KPHMT (SEQ ID NOs: 7-11, for example) Protein

Cell Growth

3 x 15 mL starting culture of E-coli Hfr3000-YA139 cells with the plasmid pCEJ01 containing the clone pAL01 was incubated at 37 °C overnight in LB broth containing ampicillin (50 mg/mL). This was added to 3 litres of LB broth containing ampicillin (50 mg/mL) and IPTG (90 mg/mL) and incubated at 37 °C for 16 h. Selenomethionine (SeMet) protein was over-expressed in media

containing selenomethionine, as well as six other amino acids (lysine, phenylalanine, threonine, isoleucine, leucine and valine) whose presence inhibit methionine biosynthesis (8) and was purified in the same way as the wild type. The cells were harvested by centrifugation at 10,000 rpm at 4 °C for 30 min. The wet cell pellet weighed approximately 9 g.

Protein Extraction

The cell pellet was resuspended in 50 mL of 100 mM phosphate buffer (pH 7) containing 1 mM DTT, 1 mM ethylenediaminetetraacetic acid (EDTA) and 1 mM phenylmethylsulphonylfluoride (PMSF). The suspension was sonicated on ice for 1 s bursts every 3 s for 12 min and the lysate centrifuged at 12,000 rpm for 30 min. Nucleic acids were removed from the supernatant by precipitation with 2% protamine sulphate (1 mL/g of cell pellet) and centrifugation at 12,000 rpm for 30 min.

The protein was precipitated from the supernatant with ammonium sulphate (25 - 60% saturation) and centrifugation at 12,000 rpm for 30 min. The protein pellet was dissolved in 30 mL of 100 mM phosphate buffer (pH 7) containing 1 mM DTT and 1 mM EDTA and dialysed, overnight against 25 mM phosphate buffer (pH 7) containing 1 mM DTT and 1 mM EDTA. The volume of the dialysed protein was reduced to below 20 mL by ultrafiltration.

Pellets that contained cell debris, 2% protamine sulphate precipitant and 0 - 25% ammonium sulphate precipitant were dissolved in a total volume of 30 mL of 100 mM phosphate buffer (pH 7) containing 1 mM DTT and 1 mM EDTA, pooled and dialysed, overnight, against 25 mM phosphate buffer (pH 7) containing 1 mM DTT and 1 mM EDTA. The volume of the dialysed mixture was reduced to below 20 mL by ultrafiltration and filtered through a 0.2 μ m filter. The protein was purified by FPLC.

Hiprep Q XL anion exchange chromatography

The sample, in less than 10 mL, was loaded, using a 10 mL superloop, onto a Hiprep 16/10 Q XL column equilibrated in starting buffer which consisted of 90% buffer A, containing 50 mM potassium phospate buffer (pH 6.9), 1 mM DDT and 1 mM EDTA, and 10% buffer B containing 50 mM potassium phosphate buffer (pH 6.9), 1 mM DDT and 1 mM EDTA and 1 M potassium chloride (KCl). KPHMT (SEQ ID NOS: 7-11, for example) was eluted in a step gradient of 0.1 - 1 M KCl in 12 column volumes (240 mL) and at a flow rate of 2.5 mL/min. The gradient was shaped as indicated below. KPHMT (SEQ ID NOS: 7-11, for example) eluted in a single peak at about 0.4 M KCl. Eluate fractions were assessed for KPHMT (SEQ ID NOS: 7-11, for example) content by SDS-PAGE. Fractions containing KPHMT (SEQ ID NOS: 7-11, for example) were pooled and dialysed overnight against starting buffer.

Source 15Q anion exchange chromatography

The sample, in less than 10 mL, was loaded, using a 10 mL superloop, onto a Source 15Q XV 16/10 column equilibrated in starting buffer which consisted of 90% buffer A, containing 25 mM potassium phospate buffer (pH 6.9), 1 mM DDT and 1 mM EDTA, and 10% buffer B containing 25 mM potassium phosphate buffer (pH 6.9), 1 mM DDT and 1 mM EDTA and 1 M KCl. KPHMT (SEQ ID NOS: 7-11, for example) was eluted of the Source 15Q XV 16/10 column in the same way it was eluted of the Hiprep 16/10 Q XL column. KPHMT (SEQ ID NOS: 7-11, for example) eluted in a single peak at about 0.4 M potassium chloride.

Eluate fractions were assessed for KPHMT (SEQ ID NOs: 7-11, for example) content by SDS-PAGE. Fractions containing KPHMT (SEQ ID NOs: 7-11, for example) were pooled and dialysed overnight against starting buffer.

KCl gradient used in anion exchange chromatography of KPHMT (SEQ ID NOs: 7-11, for example):

step 1 - 0.1 to 0.4 M KCl (0 - 50 mL)

step 2 - at 0.4 M KCl (50 - 110 mL)

step 3 - 0.4 to 0.5 M KCl (110 - 120 mL)

step 4 - at 0.5 M KCl (120 - 180 mL)

step 5 - 0.5 to 1 M KCl (180 - 190 mL)

step 6 - at 1 M KCl (190 - 240 mL)

Hiload 16/60 superdex 200 pg gel filtration chromatography

Sample was loaded in less than 10 mL onto a Hiload 16/60 superdex 200 pg equilibrated in buffer containing 50 mM potassium phosphate buffer (pH 6.9), 1 mM DDT and 1 mM EDTA. A constant flow rate of 0.5 mL per minute was maintained and 3 mL fractions were collected. Fractions containing KPHMT (SEQ ID NOs: 7-11, for example) were determined by SDS-PAGE, pooled and concentrated by ultrafiltration to greater than 5 mg/mL. 26 mg of protein was obtained from a 3 L cell culture.

2. Protein Crystallisation

The sample of KPHMT (SEQ ID NOs: 7-11, for example) was concentrated to 24 mg/ml in 40 mM of ketopantolactone (KPL; product) and 50 mM HEPES pH 7.4. Diffraction-quality single crystals of KPHMT (SEQ ID NOs: 7-11, for example) were obtained by the hanging-vapor diffusion method at 4 °C. To make a drop, one volume $(1.5 \mu l)$ of protein solution was placed on a siliconised cover slide, and the equivalent reservoir solution was added at 19 °C. Reservoir solution contained 9% (w/v) PEG 8000, 50 mM NaCitrate (pH 6.8), 50-100 mM Na(CH_3CO_2) and 200 mM NaCl. The plate was sealed within 1 minute and left at 4 °C. After 2 hours the plate was placed into a polystyrene box, then the box was sealed and placed at 19 °C. Single crystals with dimensions of about $0.5 \times 0.3 \times 0.1$ mm appeared within one or two days. These belonged to the monoclinic space group P21 with cell parameters a = 86.1 Å, b = 157.2 Å, c = 100.2 A and β = 97.4°, and accommodated one decameric enzyme per asymmetric unit, with a solvent content of 49%.

The SeMet KPHMT (SEQ ID NOs: 7-11, for example) crystals, which were prepared in a similar way to native KPHMT (SEQ ID NOs: 7-11, for example) crystals, seldom grew larger than 0.3 mm or thicker than about 30 μ m. The SeMet KPHMT (SEQ ID NOs: 7-11, for example) stock solution contained 2 mM KPL and 10 mM DTT to protect the Se atoms from oxidation.

3. Data Collection

The structure of KPHMT (SEQ ID NOs: 7-11, for example) was solved by the MAD method (9) using the SeMet derivative. Data to 3.1 Å resolution were collected at 100 K, at three wavelengths on Station 19-ID of the Structural Biology Centre at the Advanced Photon Source of Argonne National Laboratory, Chicago, US. Crystals of KPHMT (SEQ ID NOs: 7-11, for example) were cryo-protected by a protocol of gradual soaking in the cryo-protectant PEG400. Each crystal was placed in 20 ml of crystallisation solution, and the concentration of PEG400 was gradually increased to 20% (v/v) in 5% increments. The soaking time at each PEG400 concentration was a minimum of 15 minutes. At each concentration step, KPL was added to a concentration of 2 mM. The flash-cooled crystals were used for data collection.

An X-ray fluorescence spectrum was recorded and used to select wavelengths for subsequent MAD data collection. Data were collected at the Se absorption edge $\lambda e = 0.97939$ Å, the absorption peak $\lambda p = 0.97927$ Å and at remote reference wavelength $\lambda r = 0.9393$ Å. The diffraction data were indexed and integrated using the D^*TREK suite (10), and reflexions were indexed and integrated using MOSFLM (11). The three data sets were scaled to the remote data-set using SCALA (12) and structure-factor amplitudes were calculated using TRUNCATE (13). Statistics of the processed data are listed in Table 2.

The native data set was collected to 1.8 Å resolution on Station 19-ID. A cryo-protectant solution for the native crystals contained 9% PEG8000, 50 mM NaCitrate (pH 6.8), 50-100 mM Na(CH₃CO₂), 200 mM NaCl, and 20% of PEG400.

4. Structure Determination and Refinement

160 out of the 180 Se sites in the asymmetric unit were found with the program SnB (14) using direct methods and anomalous difference data of λp SeMet. Data were phased with SHARP (15) using all three wavelength data sets, which also revealed two additional Se sites in the residual maps.

Data collected at the remote wavelength were treated as the reference data set and resolution limits of 40 to 2.3 Å were imposed. Experimental values of the anomalous dispersion (f' and f'' in Table 2) estimated from fluorescence spectra were used and refined during analysis. The resulting values are very similar to the theoretical values and are given in Table 2. Experimental phases were improved by solvent flattening using SOLOMON (CCP4, 1994), via the SUSHI graphical user interface (La Fortelle et al., 1997) with a solvent content of 430%. The final electron-density map was easily interpretable and the whole polypeptide chain was assigned based on the initial electron density map.

The polypeptide chain was fitted in the MAD electron density map using program \mathcal{O} (16). Rounds of maximum likelihood refinement with REFMAC (17) were alternated with visual inspection of electron density and manual rebuilding of side chains. Several rounds of simulated annealing with CNS (18) were included to refine the position of the main chain properly.

Table 1 provides the atomic coordinates of the final model.

The quality of the final model was assessed from Ramachandran plots and the analysis of the model geometry was carried out with the program PROCHECK (19). 10% of the reflections were set aside for $R_{\mbox{free}}$ calculations. The plot indicated that 90.2% of the residues lay in the favourable regions and 9.8% in the allowed regions. The final R and $R_{\mbox{free}}$ factors of the structure for all reflections between 75.0 and 1.8 Å resolutions were 0.229 and 0.263, respectively. The structural model for KPHMT (SEQ ID NOs: 7-11, for example)

consists of a decamer in the asymmetric unit with 2,640 amino residues, 19,830 protein atoms (non-hydrogen), 100 substrate atoms (non-hydrogen), 1,612 water molecules and 10 metal ions. The last cycle of the refinement without NCS-restrains gave a reasonable stereo-chemistry by using 229,076 unique reflections in the range of 75.0 to 1.8 Å resolution. The root mean-square deviation from standard values are 0.006 Å in bond distances (1-2 distance), 1.2° in angle distances (1-3 distance), and 22.1° in dihedral angles (planar 1-4 distance). From a Ramachandran plot the model was considered to exhibit a good stereo-chemistry.

Structural Characterisation

The crystal structure of KPHMT (SEQ ID NOs: 7-11, for example) is based on a decameric asymmetric unit formed by a pentamer of dimers related by a non-crystallographic five-fold axis. Figures 3a and b show ribbon representations of the decameric structure as viewed respectively along and from the side of the non-crystallographic five-fold axis.

The dimensions of the decamer are approximately 100 x 100 x 75 Å. The accessible area of the decamer, 83,200 Ų, is small considering the surface area for each protomer (i.e. monomer subunit), 10,800 Ų, while the buried surface of each protomer is 23%. The close packing of the protomers explains the protein's remarkable resistance to denaturation by heat and urea (20). The interface between protomers in each dimeric unit is large (1140 Ų) and tightly organised, involving 88 (20 hydrophilic and 68 hydrophobic) interactions. However, the interface between protomers in the pentamer is smaller (760 Ų) and involves only 20 (6 hydrophilic and 14 hydrophobic) interactions. For this reason, we believe that the dimer is the functional unit. This is corroborated by the homologue from Aspergillus nidulans, which is an octamer (3).

Each protomer is approximately spherical and has overall dimensions of $50 \times 50 \times 40$ Å. Ribbon representation top and

side views of a protomer are presented in Figures 4c and d. The tertiary structure is an $\alpha_8\beta_8$ (TIM (triose phosphate isomerase) barrel with an extra α -helix located at the base of the β -barrel (21). The barrel consists of eight parallel β -strands surrounded by eight α -helices.

35 proteins or translated gene-sequences have been

Sequence Alignment

identified using a PSI-BLAST search, with high enough similarity to be classified as members of the KPHMT (SEQ ID NOs: 7-11, for example) family (22). The enzyme is found in bacteria, lower eukaryotes (e.g. yeast) and in the plant Arabidopsis thaliana but is not found in Caenorhabditis elegans, Drosophila melanogaster or, as yet, in other higher eukaryotes. This is consistent with the end product of this pathway being a vitamin. We have analyzed the sequences from the 35 members of this family to identify residues important to the mode of action. Correlation between primary structure among five members of the KPHMT (SEQ ID NOs: 7-11, for example) family and the secondary structure of the E. coli enzyme is shown in Figure 5 (SEQ ID NOs:7-12, respectively). The consensus sequence, generated by ClustalW (23) with the sequences of the 35 members, highlights that of the 264 residues, 23 residues are invariant while an additional 77 are conserved. Six conserved sequence motifs, at least six residues in length, were also identified. These are 42LeuValGlyAspSerLeuGlyMet49 (SEQ ID NO:1), $^{111} \text{ValLysIleGluGlyGly}^{116} \text{ (SEQ ID NO:2), } ^{135} \text{GlyHisXGlyLeuThrProGln}^{142}$ (SEQ ID NO:3) (where X is a hydrophobic residue), ¹⁴⁸GlyGlyTyrLysValGlnGly¹⁵⁴ (SEQ ID NO:4), ²⁰⁰IleGlyIleGlyAlaGly²⁰⁵ (SEQ ID NO:5) and 209AspGlyAsnIleLeuVal214 (SEQ ID NO:6). The first two of the six motifs contain residues shown in the

Deletion of residue Gly 168 (which corresponds to Gly 205 in the fifth motif given above) in A. nidulans has been shown to

crystal structure to be involved in binding the ketopantoate

(and hence the substrate) or metal ion.

prevent cell growth (3). This residue is invariant in 34 out of the 35 KPHMT (SEQ ID NOs: 7-11, for example) sequences and mutated to serine in a potentially inactive isoform from Pseudomonas aeruginosa. Thus, the motif may be required for correct folding of the protein.

Substrate Binding Site

The substrate binding site is located in a large cavity at the protein C-terminus ends of the β -strands. The cavity extends almost one quarter the distance in to the protein and is about 20 Å in length and about 10 Å x 15 Å in transverse section. The substrate is believed to bind before the cofactor, because the cofactor binds at the mouth of the cavity effectively blocking access to the cavity. Figure 6 is a stereo pair wire-frame electron density map of the substrate binding site showing a ketopantoate product molecule (KPL) and a metal ion believed to be Mg²+ on which the enzyme is dependent for its activity.

The electrostatic potential map for a protomer (shown in Figure 7) demonstrates that the opening mouth of the binding cavity is highly charged. The surface contains eight highly conserved residues that hydrogen bond to each other and the substrate or product. As shown in Figure 8, which is a stereo pair ribbon representation of the binding cavity, Asp 45 and Asp 84 hydrogen bond to Gln 142 and Lys 112, respectively, while Ser 46, Glu 181 and Lys 112 hydrogen bond to ketopantoate and the residues Tyr 25, His 136 and Asp 84.

The Mg²⁺ ion is bound in a distorted octahedral binding site of the binding cavity. Residues, Asp 45 and Asp 84 occupy axial and equatorial positions, respectively, while Glu 114 coordinates to Mg²⁺ through a water molecule that occupies an equatorial position. The keto and carboxyl groups of the product take up an axial and an equatorial position, respectively and the last equatorial position is occupied by a

water molecule. Figure 9 shows a schematic representation of the distorted octahedral binding site.

The coordination around Mg^{2+} is distorted due to hydrogen bonding between Glu 181 and the hydroxymethyl group of the product. We believe the geometry of the Mg^{2+} ion is less distorted, and hence lower in stabilization energy, when ketopantoate (product) is replaced by $\alpha\text{-KIVA}$ (substrate). This may be one mechanism by which the enzyme senses and releases the product.

Cofactor Binding Site

As yet, a $5.10-CH_2-H_4$ foliate cofactor binding motif has not been identified by X-ray crystallography. Nonetheless, we have developed an approach to find the cofactor binding site.

Initially we compared our structure to structures of tetrahydrofolate-dependent enzymes bound to folate analogues. The January, 2001 release of the Protein Data Bank (PDB) contains seven enzymes that bind tetrahydrofolate (THF). are dihydrofolate reductase (DHFR), phosphoribosylglycinamide formyltransferase (PRGF), methylenetetrahydrofolate dehydrogenase (MTDH), glycinamide ribonucleotide transformylase (GRTF), thymidylate synthase (TS), serine hydroxymethyl transferase (SHMT), and methylenetetrahydrofolate reductase (MTR). A structural similarity search by the program DALI (24) shows that only four of the above proteins appear to be similar to KPHMT (SEQ ID NOs: 7-11, for example). These are MTR, DHFR, PRGF and SHMT, but for MTR, DHFR and PRGF, the distance of the folate cofactor binding site is too far from the substrate binding site relative to the corresponding distance in KPHMT (SEQ ID NOs: 7-11, for example).

This left SHMT, which appears to be functionally similar to KPHMT (SEQ ID NOs: 7-11, for example), although SHMT is a class I aldolase (KPHMT (SEQ ID NOs: 7-11, for example) is a class II aldolase) because pyridoxal phosphate is used in addition to the folate cofactor. Given the crystal structures of SHMT from E.

coli bound to the folate, 5-formyl-THF (25) and TS bound to $5,10-CH_2-H_4$ folate or analogues thereof (26), we were able to propose a tentative model for the binding $5,10-CH_2-H_4$ folate to KPHMT (SEQ ID NOs: 7-11, for example).

Next, using multiple sequence alignment (see Figure 5) to identify residues implicated in cofactor binding, we were able to fine tune the proposed model for cofactor binding. The fine tuned model is shown in Figures 10a and b which are side and top view stereo pair ribbon representations of the mouth of the binding cavity.

In this model, $5.10-CH_2-H_4$ foliate (mTHF) binds near the entrance to the binding cavity at a depth of 15\AA . The distance between the target carbon atoms, C11 in $5.10-CH_2-H_4$ foliate and C3 in the substrate, is about 4.5\AA , a favourable distance for a reaction to occur.

The cofactor makes relatively few contacts with the protein. Interestingly, these contacts are located in regions of undefined secondary structure, namely, the loop regions that compose the entrance to the binding cavity. The loops in question are between $\beta 5$ and $\alpha 7$ (L1), $\alpha 9$ and $\alpha 10$ (L2) and the C-terminus (L3). Being regions of undefined secondary structure these loops may be highly flexible and thus, undergo structural changes upon cofactor binding. We have identified conserved residues that impart either flexibility or make strong interactions that may impart rigidity (definition) to these loops. Thus we believe that upon cofactor binding these loops undergo discrete structural changes.

Loop, L1, contains two of the six above-mentioned conserved motifs. The first half of this loop, is located deeper in the binding cavity and contains Gln 142, which H-bonds to the axial Mg²⁺ ligand, Asp 45. This half of the loop is probably rigid since it contains a turn between Asn 145 and Gly 149. The second half of the loop consists predominantly of the second motif. Both ends of this motif, namely residues Gly 148 (invariant) and Gly 154 may make this part of the loop flexible.

Gln 153 is implicated in a hydrogen bond to the amide of Lys 151, which upon cofactor binding may move to interact with the polyglutamate chain of the cofactor (see below for more discussion of this). Loop, L2, is relatively long with little sequence conservation. Invariant Gly 220 may impart some flexibility to this loop while residues Asp 217, Lys 228 and Phe 229 are implicated in binding the cofactor. In L3, invariant Pro 257 is in van der Waals contact with Gly 205 and Gln 211, while His 261 hydrogen bonds to Lys 228 and Glu 260. Thus, the deletion of Gly 168 in A. nidulans would lead to a distortion in the loop between $\beta7$ and $\beta8$ which may in turn lead to a disordering in adjacent loops such as L3 which could potentially prevent cofactor from binding. We, therefore propose that the panB auxotroph from A. nidulans is caused by the inability of the mutant KPHMT (SEQ ID NOs: 7-11, for example) enzyme to bind the cofactor and therefore to function.

There are four main protein-cofactor interactions, namely, three hydrogen bonds and a π-stacking interaction. atom at N2 of 5,10-CH2-H4folate hydrogen bonds to Asp 217, while the side chain carboxyl group of the first glutamate hydrogen bonds to the carboxyl group of Tyr 150, and Lys 228. A stronger interaction is a π-stacking or hydrophobic interaction between the p-aminobenzoic acid (PABA) ring of the cofactor and the highly conserved residues Tyr 150 and Phe 229. Tyr 150 or phenylalanine, which in this instance is a functional replacement, is found at this position in 31 out of the 35 KPHMT (SEQ ID NOs: 7-11, for example) sequences discussed above, while Phe 229 is found at this position in 34 out of the 35 KPHMT (SEQ ID NOs: 7-11, for example) sequences. Interestingly, crystal structures of the THF-dependent enzymes, TS and SHMT, with cofactor analogues bound, also implicate a π-stacking or hydrophobic interaction between the PABA ring and a tyrosine or phenylalanine (25). It would appear that nature has converged on this mechanism to bind folate cofactors.

Most folate-dependent enzymes have a higher affinity for the polyglutamate form of the folate cofactor, with the greatest increase in affinity occurring with two or three glutamate residues (27). Presumably, the polyglutamate tail increases the affinity for enzyme through interactions with surface positive charges. In the crystal structure of the bifunctional enzyme dihydrofolate reductase-thymidylate synthase from Leishmania major, the polyglutamate tail of dihydrofolate makes few specific contacts but rather is held in place by the positive charge of the local electrostatic field (28). We have identified four positive residues in KPHMT (SEQ ID NOS: 7-11, for example) that could interact with the polyglutamate tail. These are Lys 151, Arg 155 (in loop L1), Lys 231 (in loop L2) and His 261 (in loop L3).

KPHMT (SEQ ID NOs: 7-11, for example) Catalysis

KPHMT (SEQ ID NOs: 7-11, for example) catalyses the transfer of a hydroxymethyl group from cofactor (5,10-CH₂-H₄folate) to substrate (α -KIVA). The transferase reaction is an aldol reaction, namely deprotonation of the C3- carbon of α -KIVA followed by nucleophilic attack on the cofactor. The crystal structure of the apo enzyme gives insights in to the first stage in the enzyme mechanism, namely, activation of substrate and cofactor.

The C3 carbon is intrinsically acidic, through conjugation of the carboxyl and keto group, however, its acidity is enhanced by coordination of the substrate to the magnesium ion. Magnesium coordination also anchors and orients the substrate for subsequent deprotonation and nucleophilic attack. Also, the increase in distortion from octahedral geometry between substrate and product bound to the ion may be one mechanism by which the enzyme senses and releases product. The basic residue involved in abstraction of the C-3 proton of α -KIVA is believed to be Glu 181. The basicity of this residue is enhanced by a network of hydrogen bonds connecting residue Glu 181 with

residues His 136 and Lys112, which constitute an invariant triad. In the crystal structure of the apo enzyme, Glu 181 is involved in a hydrogen bond with the hydroxymethyl group of the product ketopantoate – giving rise to the greater distortion from octahedral geometry. A final role for this versatile residue is as the acid in the protonation of N10 of 5,10-CH₂-H₄folate. Kallen and Jencks (29) have concluded that the reactive component of the 5,10-CH₂-H₄folate cofactor is the iminium intermediate, formed by breakage of the C11-N10-bond and protonation of N10. This is supported by the crystal structure of TS from Lactobacillus casei where the imidazolidine ring has opened and the iminium intermediate has been hydrated (26). Thus, Glu 181 is believed to abstract a proton from α -KIVA and supply it to the cofactor.

Evidence for Cooperativity

KPHMT (SEQ ID NOs: 7-11, for example), the first enzyme in the pathway for the synthesis of pantothenic acid (see Figure 1), is inhibited by later intermediates, namely pantoate, pantothenate and CoA (1). This is most probably linked to the decameric architecture of the enzyme and involves multiple binding sites for effectors such as later pathway intermediates. All three, pantoate, pantothenate and CoA exhibit negative feedback, decreasing V_{max} , increasing K_{m} and enhancing cooperativity for the substrate. We believe we have found evidence, albeit tentative, of communication between protomers, a pre-requisite for cooperativity.

As pointed out earlier, the interface between protomers in the dimeric unit is tightly organised, involving 88 (20 hydrophilic and 68 hydrophobic) interactions. In particular one network of hydrogen bonds links the binding cavities of the vertically adjacent protomers. In the crystal structure of the apo enzyme, the products in the two vertically adjacent binding cavities are separated by only 31 Å. The H-bond network extends from ketopantoate to Ser 46 then Tyr 25 and His 68 of one

subunit to Tyr 67 then His 68 then Tyr 25 then Ser 46 and finally ketopantoate of the next subunit. In the multiple sequence alignment discussed above all residues except Tyr 67 are conserved. An interaction between Asp 26 of one subunit and His 68 of the next could replace this interaction in organisms where there is no residue at position 67 able to H-bond to His 68. The alternate H-bond network would then extend from keptanoate to Ser 46 then Tyr 25 then Asp 26 of one subunit to His 68 then Tyr 25 then Ser 46 and finally keptanoate of the next subunit (see Figure 11b which is a stereo pair ribbon representation of the binding cavities of a modified KPHMT (SEQ ID NOS: 7-11, for example) dimer).

We believe we have also identified communication between subunits within the same pentamer. This interface is close to the opening to the binding cavity, the C-terminus (loop, L3), loop, L1 and the N-terminus of the adjacent subunit (see Figure 11b which is a stereo pair ribbon representation of the interface between adjacent KPHMT (SEQ ID NOs: 7-11, for example) dimers). Binding of cofactor and substrate would affect the structure of loops, L1 and L3 and thus affect the interaction at this interface. Of particular note, is the region within loop, L1 consisting of residues Gly 138 to Glu 158. Residues, Gln 142 and Tyr 150 are respectively implicated in interacting with Mg²⁺ (indirectly) and cofactor. We have also identified a residue, Lys 151, that in the crystal structure of the apo enzyme H-bonds across the interface to Thr 5 of the adjacent dimer. We speculate that binding of cofactor will cause loop L1 to move in this region, the Lys 151 - Thr 5 interaction to break, and a new interaction between Lys 151 and the polyglutamate tail of the cofactor to form.

Structure-Based Drug Design

Determination of the 3D structure of KPHMT (SEQ ID NOs: 7-11, for example) provides important information about the binding sites of KPHMT (SEQ ID NOs: 7-11, for example), particularly when comparisons are made with similar enzymes. This information may then be used for rational design of KPHMT (SEQ ID NOs: 7-11, for example) inhibitors, e.g. by computational techniques which identify possible binding ligands for the binding sites, by enabling linked-fragment approaches to drug design, and by enabling the identification and location of bound ligands using X-ray crystallographic analysis. These techniques are discussed in more detail below.

Greer et al. describes an iterative approach to ligand design based on repeated sequences of computer modelling, protein-ligand complex formation and X-ray crystallographic or NMR spectroscopic analysis. Thus novel thymidylate synthase inhibitor series were designed de novo by Greer et al., and KPHMT (SEQ ID NOs: 7-11, for example) inhibitors may also be designed in the this way. More specifically, using e.g. GRID on the solved 3D structure of KPHMT (SEQ ID NOs: 7-11, for example), a ligand (e.g. a potential inhibitor) for KPHMT (SEQ ID NOs: 7-11, for example) may be designed that complements the functionalities of the KPHMT (SEQ ID NOs: 7-11, for example) binding site(s). The ligand can then be synthesised, formed into a complex with KPHMT (SEQ ID NOs: 7-11, for example), and the complex then analysed by X-ray crystallography to identify the actual position of the bound ligand. The structure and/or functional groups of the ligand can then be adjusted, if necessary, in view of the results of the X-ray analysis, and the synthesis and analysis sequence repeated until an optimised ligand is obtained. Related approaches to structure-based drug design are also discussed in Bohacek et al., Medicinal Research Reviews, Vol.16, (1996), 3-50.

As a result of the determination of the KPHMT (SEQ ID NOs: 7-11, for example) 3D structure, more purely computational techniques for rational drug design may also be used to design KPHMT (SEQ ID NOs: 7-11, for example) inhibitors (for an overview of these techniques see e.g. Walters et al.). For example, automated ligand-receptor docking programs (discussed

e.g. by Jones et al. in Current Opinion in Biotechnology, Vol.6, (1995), 652-656) which require accurate information on the atomic coordinates of target receptors may be used to design potential KPHMT (SEQ ID NOs: 7-11, for example) inhibitors.

Linked-fragment approaches to drug design also require accurate information on the atomic coordinates of target receptors. The basic idea behind these approaches is to determine (computationally or experimentally) the binding locations of plural ligands to a target molecule, and then construct a molecular scaffold to connect the ligands together in such a way that their relative binding positions are The connected ligands thus form a potential lead compound that can be further refined using e.g. the iterative technique of Greer et al.. For a virtual linked-fragment approach see Verlinde et al., J. of Computer-Aided Molecular Design, 6, (1992), 131-147, and for NMR and X-ray approaches see Shuker et al., Science, 274, (1996), 1531-1534 and Stout et al., Structure, 6, (1998), 839-848. The use of these approaches to design KPHMT (SEQ ID NOs: 7-11, for example) inhibitors is made possible by the determination of the KPHMT (SEQ ID NOs: 7-11, for example) structure.

Many of the techniques and approaches to structure-based drug design described above rely at some stage on X-ray analysis to identify the binding position of a ligand in a ligand-protein complex. A common way of doing this is to perform X-ray crystallography on the complex, produce a difference Fourier electron density map, and associate a particular pattern of electron density with the ligand. However, in order to produce the map (as explained e.g. by Blundell et al.) it is necessary to know beforehand the protein 3D structure (or at least the protein structure factors). Therefore, determination of the KPHMT (SEQ ID NOS: 7-11, for example) structure also allows difference Fourier electron density maps of KPHMT (SEQ ID NOS: 7-11, for example)—ligand complexes to be produced, which can greatly assist the process of rational drug design.

The approaches to structure-based drug design described above all require initial identification of possible compounds for interaction with target bio-molecule (in this case KPHMT (SEQ ID NOs: 7-11, for example)). Sometimes these compounds are known e.g. from the research literature. However, when they are not, or when novel compounds are wanted, a first stage of the drug design program may involve computer-based in silico screening of compound databases (such as the Cambridge Structural Database) with the aim of identifying compounds which interact with the binding site or sites of the target biomolecule. Screening selection criteria may be based on pharmacokinetic properties such as metabolic stability and toxicity. However, determination of the KPHMT (SEQ ID NOs: 7-11, for example) structure allows the architecture and chemical nature of each KPHMT (SEQ ID NOs: 7-11, for example) binding site to be identified, which in turn allows the geometric and functional constraints of a descriptor for the potential inhibitor to be derived. The descriptor is, therefore, a type of virtual 3-D pharmacophore, which can also be used as selection criteria or filter for database screening.

While the invention has been described in conjunction with the exemplary embodiments described above, many equivalent modifications and variations will be apparent to those skilled in the art when given this disclosure. Accordingly, the exemplary embodiments of the invention set forth are considered to be illustrative and not limiting. Various changes to the described embodiments may be made without departing from the spirit and scope of the invention.

The references in the above text and listed below are incorporated by reference.

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TABLE 1

```
REMARK coordinates from minimization and B-factor refinement
REMARK refinement resolution: 500.0 - 1.8 A
REMARK starting r= 0.2289 free_r= 0.2635
REMARK final r= 0.2292 free_r= 0.2638
REMARK rmsd bonds= 0.005641 rmsd angles= 1.11562
REMARK B rmsd for bonded mainchain atoms= 1.325 target= 1.5
REMARK B rmsd for bonded sidechain atoms= 2.001 target= 2.0
REMARK B rmsd for angle mainchain atoms= 2.071 target= 2.0
REMARK B rmsd for angle sidechain atoms= 2.863 target= 2.5
REMARK target= mlf final wa= 1.10321
REMARK final rweight= 0.0678 (with wa= 1.10321)
REMARK md-method= torsion annealing schedule= constant
REMARK starting temperature= 1000 total md steps= 1 * 100
REMARK cycles= 2 coordinate steps= 20 B-factor steps= 10
REMARK sg= P2(1) a= 86.074 b= 157.17 c= 100.181 alpha= 90 beta= 97.44 gamma= 90
REMARK topology file 1 : CNS_TOPPAR:protein.top
REMARK topology file 2 : CNS_TOPPAR:dna-rna.top
REMARK topology file 3 : CNS_TOPPAR:water.top
REMARK topology file 4 : CNS_TOPPAR:ion.top
REMARK topology file 5 : ./TOPH_PARAM/kpl.toph
REMARK parameter file 1 : CNS_TOPPAR:protein_rep.param
REMARK parameter file 2 : CNS_TOPPAR:dna-rna_rep.param
REMARK parameter file 3 : CNS_TOPPAR:water_rep.param
REMARK parameter file 4 : CNS_TOPPAR:ion.param
REMARK parameter file 5 : ./TOPH_PARAM/kpl.param
REMARK molecular structure file: generate.mtf
REMARK input coordinates: generate.pdb
REMARK reflection file= ./int/panb.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.8
REMARK initial B-factor correction applied to fobs :
REMARK B11= -1.301 B22= -2.124 B33= 3.425
REMARK B12= 0.000 B13= 1.230 B23= 0.000
                                                    3.425
REMARK B-factor correction applied to coordinate array B:
                                                                           0.254
REMARK bulk solvent: density level= 0.392735 e/A^3, B-factor= 64.4356 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range:
                                                                            243384 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |\bar{F}|=0): 14308 (
                                                                                           5.9 %)
REMARK number of reflections rejected:
                                                                                  0 (
                                                                                           0.0 %)
                                                                             229076 ( 94.1 % )
REMARK total number of reflections used:
REMARK number of reflections in working set:
                                                                             206168 (
                                                                                         84.7 % )
REMARK number of reflections in test set:
                                                                              22908 (
                                                                                         9.4 %)
CRYST1 86.074 157.170 100.181 90.00 97.44 90.00 P 21 REMARK FILENAME="refine.pdb"
REMARK DATE:17-Oct-00 01:40:10
                                              created by user: inouet
REMARK VERSION:1.0
                                       1.201 12.262 69.884 1.00 67.43
MOTA
            1 CB MET
                                         0.767 11.220 70.906 1.00 69.43
1.582 11.428 72.507 1.00 72.24
ATOM
            2 CG MET
                               1
ATOM
               SD MET
            3
                                         3.012 10.336 72.306 1.00 71.04
            4 CE MET
MOTA
                               1
                                         1.282 10.813 67.848 1.00 63.63
2.165 10.936 66.998 1.00 63.58
            5 C MET
6 O MET
MOTA
                               1
MOTA
                               1
MOTA
            7 N MET
                               1
                                        -0.854 11.909
                                                            68.546 1.00 65.98
            8 CA MET
                                        0.631 12.042
                                                            68.480 1.00 65.57
MOTA
                               1
                                                  9.631 68.271 1.00 61.39
MOTA
            9 N LYS
                               2
                                        0.841
                                                  8.379 67.750 1.00 58.18
7.518 68.886 1.00 59.31
MOTA
                                        1.376
           10 CA LYS
                               2
MOTA
           11 CB LYS
                               2
                                         1.946
MOTA
                                        3.141 8.121 69.610 1.00 60.51
           12 CG
                     LYS
MOTA
           13 CD
                     LYS
                               2
                                         3.805
                                                   7.096
                                                            70.523 1.00 61.39
                                                  6.572 71.585 1.00 62.31
ATOM
           14 CE LYS
                               2
                                         2.844
                                         3.441
0.313
ATOM
                                                   5.457 72.377
                                                                      1.00 62.32
           15 NZ LYS
                               2
                                                   7.577 67.003 1.00 54.66
MOTA
           16
               C
                     LYS
                               2
MOTA
           17
                0
                     LYS
                               2
                                       -0.258
                                                  6.631 67.548 1.00 55.68
                                                                      1.00 50.09
ATOM
           18 N
                     PRO
                               3
                                        0.021
                                                   7.953 65.749
                                                  7.007 64.792 1.00 49.24
               CD
                                        -0.580
АТОМ
                     PRO
                               3
           19
                                                  9.074 65.034 1.00 45.89
8.501 63.644 1.00 47.20
MOTA
           20 CA
                     PRO
                               3
                                        0.633
MOTA
           21
                     PRO
                               3
                                        0.847
                CB
                                                  7.717 63.455 1.00 47.74
MOTA
           22 CG PRO
                               3
                                        -0.403
                                       -0.291 10.290 65.014
-1.403 10.253 65.547
           23 C
24 O
                                                                      1.00 41.96
MOTA
                     PRO
                               3
                                                                      1.00 40.18
ATOM
                     PRO
                               3
                                       0.175 11.363 64.389 1.00 37.27
-0.605 12.586 64.284 1.00 33.03
0.316 13.808 64.214 1.00 32.00
MOTA
           25 N
                     THR
                               4
MOTA
           26
                CA
                     THR
                               4
                CB
MOTA
           27
                     THR
MOTA
                                        1.113 13.866 65.403 1.00 29.60
           28 OG1 THR
```

| ATOM | 29 | CG2 | THR | 4 | -0.496 | 15.084 | 64.077 | 1.00 30.09 |
|--------------|----------|---------|------------|--------|------------------|------------------|------------------|--------------------------|
| MOTA | 30 | С | THR | 4 | -1.436 | 12.516 | 63.012 | 1.00 31.90 |
| MOTA | 31 | 0 | THR | 4 | -0.890 | 12.415 | 61.917 | 1.00 31.80 |
| MOTA | 32 | N | THR | 5 | -2.755 | 12.574 | 63.156 | 1.00 30.88 |
| MOTA | 33 | CA | THR | 5 | -3.636 | 12.494 | 61.999 | 1.00 29.95 |
| MOTA | 34 | CB | THR | 5 | -4.616 | 11.320 | 62.137 | 1.00 30.13 |
| ATOM , | 35 | OG1 | THR | 5 | -5.545 | 11.602 | 63.189 | 1.00 31.18 |
| MOTA | 36 | CG2 | THR | 5 | -3.864 | 10.035 | 62.462 | 1.00 29.84 |
| MOTA | 37 | С | THR | 5 | -4.445 | 13.764 | 61.789 | 1.00 28.70 |
| MOTA | 38 | 0 | THR | 5 | -4.407 | 14.684 | 62.605 | 1.00 28.11 |
| ATOM | 39 | N | ILE | 6 | -5.184 | 13.804 | 60.685 | 1.00 28.91 |
| ATOM | 40 | CA | ILE | 6 | -6.009 | 14.961 | 60.360 | 1.00 29.62 |
| MOTA | 41 | CB | ILE | 6 | -6.777 | 14.749 | 59.042 | 1.00 30.80 |
| ATOM | 42 | CG2 | ILE | 6 | -7.445 | 16.047 | 58.617 | 1.00 29.12 |
| MOTA | 43 | CG1 | ILE | 6 | -5.813 | 14.298 | 57.945 | 1.00 33.13 |
| ATOM | 44 | CD1 | | 6 | -6.513 | 13.840 | 56.671 | 1.00 34.94 |
| MOTA | 45 | С | ILE | 6 | -7.016 | 15.189 | 61.477 | 1.00 29.79 |
| ATOM | 46 | О | ILE | 6 | -7.339 | 16.327 | 61.813 | 1.00 30.34 |
| ATOM | 47 | N | SER | 7 | -7.499 | 14.091 | 62.051 | 1.00 29.76 |
| MOTA | 48 | CA | SER | 7 | -8.474 | 14.142 | 63.138 | 1.00 30.44 |
| ATOM | 49 | CB | SER | 7 | -8.748 | 12.730 | 63.653 | 1.00 31.47 |
| ATOM | 50 | OG | SER | 7 | -8.920 | 11.822 | 62.575 | 1.00 37.31 |
| MOTA | 51 | C | SER | 7 | -7.954 | 15.006 | 64.285 | 1.00 29.13 |
| MOTA | 52 | 0 | SER | 7 | -8.712 | 15.751 | 64.909 | 1.00 28.63 |
| ATOM | 53 | N | LEU | 8 | -6.655 | 14.902 | 64.556 | 1.00 27.78 |
| ATOM | 54 | CA | LEU | 8 | -6.035 | 15.668 | 65.630 | 1.00 27.46 |
| ATOM | 55 | CB | LEU | 8 | -4.553 | 15.296 | 65.778 | 1.00 28.11 |
| ATOM | 56 | CG | LEU | 8 | -3.954 | 15.254 | 67.190 | 1.00 30.83 |
| ATOM | 57 | | LEU | 8 | -2.452 | 15.499 | 67.105 | 1.00 30.15 |
| ATOM | 58 | | LEU | 8 | -4.594 | 16.302 | 68.086 | 1.00 32.65 1.00 26.61 |
| ATOM | 59 | C | LEU | 8 | -6.141 | 17.173 | 65.378 | 1.00 26.61 |
| ATOM | 60 | 0 | LEU | 8 9 | -6.388 -5.951 | 17.943 17.589 | 66.303 64.129 | 1.00 28.41 |
| ATOM ATOM | 61 62 | N CA | LEU LEU | 9 | -6.024 | 19.005 | 63.799 | 1.00 24.65 |
| ATOM | 63 | CB | LEU | 9 | -5.388 | 19.279 | 62.431 | 1.00 24.03 |
| ATOM | 64 | CG | LEU | 9 | -3.926 | 18.838 | 62.239 | 1.00 22.20 |
| ATOM | 65 | | LEU | 9 | -3.403 | 19.371 | 60.914 | 1.00 13.32 |
| ATOM | 66 | | LEU | 9 | -3.076 | 19.367 | 63.382 | 1.00 18.44 |
| ATOM | 67 | C | LEU | 9 | -7.468 | 19.500 | 63.805 | 1.00 26.68 |
| ATOM | 68 | 0 | LEU | 9 | -7.737 | 20.650 | 64.151 | 1.00 26.46 |
| ATOM | 69 | N | GLN | 10 | -8.396 | 18.627 | 63.426 | 1.00 29.15 |
| ATOM | 70 | CA | GLN | 10 | -9.808 | 18.990 | 63.403 | 1.00 32.76 |
| ATOM | 71 | CB | GLN | 10 | -10.632 | 17.869 | 62.764 | 1.00 32.40 |
| ATOM | 72 | CG | GLN | 10 | -12.091 | 18.220 | 62.511 | 1.00 34.98 |
| ATOM | 73 | CD | GLN | 10 | | 19.495 | 61.698 | 1.00 34.51 |
| ATOM | 74 | | GLN | 10 | -12.158 | 20.601 | 62.228 | 1.00 35.90 |
| ATOM | 75 | | GLN | 10 | -12.518 | 19.343 | 60.403 | 1.00 33.91 |
| ATOM | 76 | С | GLN | 10 | -10.256 | 19.239 | 64.841 | 1.00 34.38 |
| ATOM | 77 | Ο. | GLN | 10 | -11.132 | 20.066 | 65.093 | 1.00 35.73 |
| ATOM | 78 | N | LYS | 11 | -9.640 | 18.528 | 65.781 | 1.00 36.20 |
| ATOM | 79 | CA | LYS | 11 | -9.961 | 18.694 | 67.193 | 1.00 37.50 |
| ATOM | 80 | CB | LYS | 11 | -9.374 | 17.548 | 68.023 | 1.00 39.71 |
| MOTA | 81 | CG | LYS | 11 | -9.466 | 17.788 | 69.526 | 1.00 42.23 |
| MOTA | 82 | CD | LYS | 11 | -8.571 | 16.850 | 70.326 | 1:00 45.49 |
| MOTA | 83 | CE | LYS | 11 | -9.131 | 15.436 | 70.387 | 1.00 47.75 |
| MOTA | 84 | NZ | LYS | 11 | -8.313 | 14.563 | 71.283 | 1.00 48.44 |
| MOTA | 85 | С | LYS | 11 | -9.378 | 20.016 | 67.677 | 1.00 37.17 |
| ATOM | 86 | 0 | LYS | 11 | -9.988 | 20.721 | 68.483 | 1.00 38.57 |
| ATOM | 87 | N | TYR | 12 | -8.189 | 20.345 | 67.181 | 1.00 36.59 |
| ATOM | 88 | CA | TYR | 12 | -7.512 | 21.585 | 67.548 | 1.00 35.53 |
| MOTA | 89 | CB | TYR | 12 | -6.145 | 21.665 | 66.864 | 1.00 36.51 |
| MOTA | 90 | CG | TYR | 12 | -5.070 | 20.803 | 67.486 | 1.00 37.30 |
| MOTA | 91 | CD1 | | 12 | -3.889 | 20.534 | 66.797 | 1.00 38.03 |
| MOTA | 92 | CE1 | TYR | 12 | -2.880 | 19.769 | 67.371 | 1.00 38.86 |
| ATOM | 93 | CD2 | TYR | 12 | -5.217 | 20.281 | 68.772 | 1.00 37.36 |
| ATOM | 94 | CE2 | TYR | 12 | -4.213 | 19.515 | 69.356 | 1.00 38.58 |
| ATOM | 95 | CZ | TYR | 12 | -3.047 | 19.264 | 68.648 | 1.00 39.25 |
| ATOM | 96 | ОН | TYR | 12 | -2.044 | 18.514 | 69.220 | 1.00 40.19 |
| ATOM | 97 | С | TYR | 12 | -8.324 | 22.815 | 67.169 | 1.00 34.82 |
| ATOM | 98 | 0 | TYR | 12 | -8.451 | 23.748 | 67.960 | 1.00 34.13 |
| ATOM | 99 | N | LYS | 13 | -8.860 | 22.822 | 65.953 | 1.00 34.10 |
| ATOM | 100 | CA | LYS | 13 | -9.652 | 23.960 | 65.496 | 1.00 35.74 |
| MOTA | 101 | CB | LYS | 13 | -10.087 | 23.765 | 64.041 | 1.00 34.52 |
| MOTA | 102 | CG | LYS | 13 | -10.895 | 24.927 | 63.458 | 1.00 34.21 |
| ATOM | 103 | CD | LYS | 13 | -11.268 | 24.645 | 62.001 | 1.00 31.63 |
| MOTA | 104 | CE | LYS | 13 | -12.274 | 25.645 | | 1.00 31.85 |
| MOTA | 105 | NZ | LYS | 13 | -11.675 | 26.929 | 60.984 | 1.00 30.98 |

| ATOM | 106 | С | LYS | 13 | -10.878 | 24.124 | 66.385 | 1.00 | 36.28 |
|-------|-----|-----|------|----|---------|---------|--------|------|-------|
| ATOM | 107 | 0 | LYS | 13 | -11.336 | 25.240 | 66.622 | 1.00 | 34.68 |
| ATOM | 108 | N | GLN | 14 | -11.404 | 23.004 | 66.869 | | 38.20 |
| | 109 | CA | GLN | 14 | -12.572 | 23.018 | 67.744 | | 40.77 |
| ATOM | 110 | CB | GLN | 14 | -13.049 | 21.591 | 68.007 | | 42.50 |
| ATOM | | | | | | | | | |
| MOTA | 111 | CG | GLN | 14 | -13.662 | 20.906 | 66.800 | | 47.11 |
| ATOM | 112 | CD | GLN. | 14 | -13.789 | 19.407 | 66.992 | | 49.44 |
| ATOM | 113 | OE1 | GLN | 14 | -14.221 | 18.939 | 68.046 | | 51.52 |
| MOTA | 114 | NE2 | GLN | 14 | -13.419 | 18.645 | 65.967 | 1.00 | 50.79 |
| MOTA | 115 | C | GLN | 14 | -12.227 | 23.688 | 69.071 | 1.00 | 40.73 |
| ATOM | 116 | 0 | GLN | 14 | -13.043 | 24.409 | 69.648 | 1.00 | 40.91 |
| ATOM | 117 | N | GLU | 15 | -11.010 | 23.443 | 69.545 | 1.00 | 39.66 |
| ATOM | 118 | CA | GLU | 15 | -10.544 | 24.008 | 70.805 | | 39.32 |
| ATOM | 119 | СВ | GLU | 15 | -9.544 | 23.054 | 71.465 | | 40.94 |
| | 120 | CG | GLU | 15 | -10.012 | 21.607 | 71.509 | | 43.66 |
| ATOM | | | | | | | | | 44.96 |
| ATOM | 121 | CD | GLU | 15 | -9.013 | 20.679 | 72.180 | | |
| ATOM | 122 | OE1 | | 15 | -7.834 | 20.658 | 71.768 | | 44.85 |
| ATOM | 123 | OE2 | GLU | 15 | -9.409 | 19.959 | 73.121 | | 48.88 |
| ATOM | 124 | С | GLU | 15 | -9.880 | 25.357 | 70.567 | 1.00 | 38.67 |
| ATOM | 125 | 0 | GLU | 15 | -9.381 | 25.985 | 71.502 | 1.00 | 38.21 |
| ATOM | 126 | N | LYS | 16 | -9.889 | 25.803 | 69.313 | 1.00 | 37.45 |
| ATOM | 127 | CA | LYS | 16 | -9.269 | 27.069 | 68.939 | 1.00 | 36.93 |
| ATOM | 128 | CB | LYS | 16 | -9.957 | 28.235 | 69.655 | | 39.24 |
| ATOM | 129 | CG | LYS | 16 | -10.820 | 29.105 | 68.748 | | 42.46 |
| | 130 | CD | LYS | 16 | -9.963 | 29.912 | 67.783 | | 44.77 |
| ATOM | | | | | | 30.700 | 66.794 | | 45.69 |
| ATOM | 131 | CE | LYS | 16 | -10.809 | | | | |
| ATOM | 132 | ΝŻ | LYS | 16 | -11.734 | 31.653 | 67.466 | | 45.98 |
| ATOM | 133 | С | LYS | 16 | -7.777 | 27.055 | 69.272 | | 35.34 |
| ATOM` | 134 | 0 | LYS | 16 | -7.170 | 28.103 | 69.507 | | 34.70 |
| ATOM | 135 | N | LYS | 17 | -7.186 | 25.865 | 69.304 | 1.00 | 33.29 |
| ATOM | 136 | CA | LYS | 17 | -5.759 | 25.752 | 69.593 | 1.00 | 32.28 |
| ATOM | 137 | CB | LYS | 17 | -5.440 | 24.423 | 70.285 | 1.00 | 34.01 |
| ATOM | 138 | CG | LYS | 17 | -3.951 | 24.238 | 70.580 | 1.00 | 36.37 |
| ATOM | 139 | CD | LYS | 17 | -3.618 | 22.820 | 71.033 | | 39.39 |
| ATOM | 140 | CE | LYS | 17 | | 22.504 | 72.405 | | 41.80 |
| | | | | 17 | -3.935 | 21.089 | 72.804 | | 42.95 |
| ATOM | 141 | NZ | LYS | | | | | | |
| ATOM | 142 | С | LYS | 17 | -4.955 | 25.854 | 68.298 | | 30.45 |
| MOTA | 143 | 0 | LYS | 17 | -4.935 | 24.923 | 67.495 | | 29.95 |
| MOTA | 144 | N | ARG | 18 | -4.299 | 26.993 | 68.103 | | 28.24 |
| MOTA | 145 | CA | ARG | 18 | -3.486 | 27.224 | 66.913 | | 27.71 |
| MOTA | 146 | CB | ARG | 18 | -3.084 | 28.693 | 66.841 | | 26.93 |
| ATOM | 147 | CG | ARG | 18 | -4.213 | .29.588 | 66.366 | 1.00 | 29.98 |
| ATOM | 148 | CD | ARG | 18 | -3.904 | 31.058 | 66.576 | 1.00 | 31.56 |
| ATOM | 149 | NE | ARG | 18 | -3.975 | 31.427 | 67.989 | 1.00 | 33.11 |
| ATOM | 150 | CZ | ARG- | 18 | -3874 | 32.673 | 68.437 | 1.00 | 34.92 |
| ATOM | 151 | | ARG | 18 | -3.694 | 33.671 | 67.580 | | 34.93 |
| ATOM | 152 | NH2 | ARG | 18 | -3.961 | 32.921 | 69.736 | | 33.10 |
| | 153 | C | ARG | 18 | -2.249 | 26.329 | 66.912 | | 26.09 |
| ATOM | | | | | | | | | |
| ATOM | 154 | 0 | ARG | 18 | -1.455 | 26.357 | 67.852 | | 27.27 |
| ATOM | 155 | N | PHE | 19 | -2.093 | 25.546 | 65.845 | 1.00 | 24.65 |
| MOTA | 156 | CA | PHE | 19 | -0.983 | 24.601 | 65.710 | | 21.83 |
| ATOM | 157 | CB | PHE | 19 | -1.543 | 23.213 | 65.386 | | |
| ATOM | 158 | CG | PHE | 19 | -2.394 | 23.176 | 64.147 | | 21.17 |
| ATOM | 159 | CD1 | PHE | 19 | -1.813 | 23.054 | 62.885 | 1.00 | 21.71 |
| ATOM | 160 | CD2 | PHE | 19 | -3.779 | 23.275 | 64.240 | 1.00 | 21.90 |
| ATOM | 161 | CE1 | PHE | 19 | -2.604 | 23.036 | 61.730 | 1.00 | 20.83 |
| ATOM | 162 | | PHE | 19 | -4.582 | 23.259 | 63.095 | 1.00 | 20.74 |
| ATOM | 163 | CZ | PHE | 19 | -3.995 | 23.137 | 61.837 | | 22.45 |
| ATOM | 164 | C | PHE | 19 | 0.075 | 24.985 | 64.678 | | 20.64 |
| ATOM | 165 | o | PHE | 19 | -0.208 | 25.687 | 63.708 | | 20.24 |
| | 166 | | | 20 | 1.298 | 24.509 | 64.894 | | 17.95 |
| MOTA | | N | ALA | | | | | | |
| MOTA | 167 | CA | ALA | 20 | 2.409 | 24.801 | 63.994 | | 18.49 |
| ATOM | 168 | CB | ALA | 20 | 3.671 | 25.051 | 64.808 | | 16.95 |
| MOTA | 169 | С | ALA | 20 | 2.676 | 23.705 | 62.959 | | 17.84 |
| MOTA | 170 | 0 | ALA | 20 | 2.563 | 22.515 | 63.253 | | 19.20 |
| MOTA | 171 | N | THR | 21 | 3.035 | 24.126 | 61.750 | | 19.33 |
| ATOM | 172 | CA | THR | 21 | 3.351 | 23.211 | 60.654 | 1.00 | 21.03 |
| ATOM | 173 | CB | THR | 21 | 2.235 | 23.215 | 59.595 | 1.00 | 22.40 |
| ATOM | 174 | | THR | 21 | 1.013 | 22.766 | 60.201 | | 25.51 |
| ATOM | 175 | CG2 | | 21 | 2.583 | 22.298 | 58.449 | | 28.47 |
| ATOM | 176 | C | THR | 21 | 4.667 | 23.668 | 60.022 | | 18.87 |
| ATOM | 177 | o | THR | 21 | 5.028 | 24.846 | 60.095 | | 19.63 |
| | | | | | 5.391 | | 59.387 | | 17.33 |
| ATOM | 178 | N | ILE | 22 | | 22.757 | | | |
| ATOM | 179 | CA | ILE | 22 | 6.672 | 23.156 | 58.822 | | 16.75 |
| ATOM | 180 | CB | ILE | 22 | 7.761 | 23.058 | 59.915 | | 16.67 |
| ATOM | 181 | CG2 | ILE | 22 | 8.068 | 21.593 | 60.208 | | 16.67 |
| MOTA | 182 | CG1 | ILE | 22 | 9.009 | 23.833 | 59.492 | 1.00 | 18.38 |

| ATOM | 183 | CD1 | ILE | 22 | | 9.959 | 24.160 | 60.653 | 1.00 | 19.13 |
|------|------|-----|-------|----|---|----------|--------|--------|------|-------|
| ATOM | 184 | С | ILE | 22 | | 7.068 | 22.314 | 57.617 | 1.00 | 16.22 |
| MOTA | 185 | 0 | ILE | 22 | | 6.592 | 21.194 | 57.459 | 1.00 | 16.81 |
| ATOM | 186 | N | THR | 23 | | 7.911 | 22.868 | 56.754 | 1.00 | 15.76 |
| ATOM | 187 | CA | THR | 23 | | 8.357 | 22.119 | 55.586 | 1.00 | 19.36 |
| ATOM | 188 | CB | THR | 23 | | 8.756 | 23.061 | 54.409 | 1.00 | 18.72 |
| MOTA | 189 | OG1 | THR | 23 | | 10.010 | 23.697 | 54.692 | 1.00 | 23.35 |
| ATOM | 190 | CG2 | THR | 23 | | 7.699 | 24.155 | 54.216 | 1.00 | 23.17 |
| MOTA | 191 | С | THR | 23 | | 9.564 | 21.285 | 56.014 | 1.00 | 18.45 |
| MOTA | 192 | 0 | THR | 23 | | 10.274 | 21.643 | 56.954 | 1.00 | 18.13 |
| MOTA | 193 | N | ALA | 24 | | 9.772 | 20.155 | 55.343 | 1.00 | 17.71 |
| ATOM | 194 | CA | ALA | 24 | | 10.897 | 19.276 | 55.633 | 1.00 | 16.52 |
| MOTA | 195 | СВ | ALA | 24 | | 10.575 | 18.345 | 56.796 | 1.00 | 16.73 |
| MOTA | 196 | C | ALA | 24 | | 11.132 | 18.483 | 54.358 | 1.00 | 15.72 |
| ATOM | 197 | Ō | ALA | 24 | | 10.181 | 18.183 | 53.634 | | 13.61 |
| ATOM | 198 | N | TYR | 25 | | 12.387 | 18.148 | 54.079 | | 15.44 |
| ATOM | 199 | CA | TYR | 25 | | 12.713 | 17.420 | 52.859 | | 15.30 |
| ATOM | 200 | CB | TYR | 25 | | 13.205 | 18.389 | 51.780 | | 16.75 |
| ATOM | 201 | CG. | TYR | 25 | | 12.454 | 19.697 | 51.729 | | 19.07 |
| ATOM | 202 | CD1 | | 25 | | 12.934 | 20.822 | 52.402 | 1.00 | 17.12 |
| ATOM | 203 | CE1 | TYR | 25 | | 12.240 | 22.026 | 52.379 | 1.00 | 22.53 |
| ATOM | 204 | CD2 | | 25 | | 11.255 | 19.808 | 51.028 | | 17.14 |
| ATOM | 205 | CE2 | | 25 | | 10.546 | 21.010 | 50.999 | | 21.05 |
| ATOM | 206 | CZ | TYR | 25 | | 11.044 | 22.114 | 51.678 | | 22.44 |
| ATOM | 207 | ОН | TYR | 25 | | 10.347 | 23.300 | 51.669 | | 25.31 |
| ATOM | 208 | C | TYR | 25 | | 13.785 | 16.359 | 53.068 | | 17.26 |
| ATOM | 209 | ō | TYR | 25 | | 14.327 | 15.837 | 52.094 | | 16.21 |
| ATOM | 210 | N | ASP | 26 | | 14.101 | 16.051 | 54.320 | | 15.99 |
| ATOM | 211 | CA | ASP | 26 | , | 15.121 | 15.059 | 54.604 | | 16.04 |
| ATOM | 212 | CB | ASP | 26 | | 16.511 | 15.686 | 54.453 | | 14.69 |
| ATOM | 213 | CG | ASP | 26 | | 16.803 | 16.751 | 55.507 | | 16.04 |
| | .214 | | ASP | 26 | | 17.002 | 16.391 | 56.679 | | 17.13 |
| ATOM | 215 | | ASP | 26 | | 16.829 | 17.935 | 55.144 | 1.00 | 14.58 |
| ATOM | 216 | C | ASP | 26 | | 14.967 | 14.426 | 55.981 | | 16.01 |
| ATOM | 217 | ō | ASP | 26 | | 14.182 | 14.888 | 56.813 | | 16.69 |
| ATOM | 218 | N | TYR | 27 | | - 15.718 | 13.353 | 56.214 | | 13.50 |
| ATOM | 219 | CA | TYR | 27 | | 15.660 | 12.625 | 57.474 | | 15.85 |
| ATOM | 220 | СВ | TYR | 27 | | 16.591 | 11.412 | 57.408 | 1.00 | 16.76 |
| ATOM | 221 | CG | TYR | 27 | | 16.777 | 10.693 | 58.727 | 1.00 | 17.84 |
| ATOM | 222 | | TYR | 27 | | 15.871 | 9.723 | 59.150 | | 17.06 |
| ATOM | 223 | | TYR | 27 | | 16.053 | 9.046 | 60.353 | | 18.09 |
| ATOM | 224 | | TYR | 27 | | 17.873 | 10.975 | 59.546 | | 19.28 |
| ATOM | 225 | | TYR | 27 | | 18.065 | 10.311 | 60.748 | 1.00 | 20.21 |
| ATOM | 226 | CZ | TYR | 27 | | 17.163 | 9.350 | 61.151 | | 20.97 |
| ATOM | 227 | ОН | TYR | 27 | | 17.368 | 8.691 | 62.342 | | 21.54 |
| ATOM | 228 | С | TYR | 27 | | 16.056 | 13.482 | 58.671 | | 15.76 |
| ATOM | 229 | ō | TYR | 27 | | 15.338 | 13.544 | 59.670 | | 16.46 |
| ATOM | 230 | N | SER | 28 | | 17.216 | 14.121 | 58.560 | | 16.97 |
| ATOM | 231 | ·CA | SER | 28 | | 17.763 | 14.943 | 59.630 | | 17.00 |
| ATOM | 232 | СВ | SER | 28 | | 19.034 | 15.643 | 59.146 | 1.00 | 19.12 |
| ATOM | 233 | OG | SER | 28 | | 20.029 | 14.671 | 58.842 | | 22.00 |
| ATOM | 234 | C | SER | 28 | | 16.798 | 15.957 | 60.222 | | 17.23 |
| ATOM | 235 | ō | SER | 28 | | 16.485 | 15.905 | 61.422 | | 16.02 |
| ATOM | 236 | N | PHE | 29 | | 16.307 | 16.881 | 59.408 | | 15.80 |
| ATOM | 237 | CA | PHE | 29 | | 15.382 | 17.864 | 59.965 | | 16.28 |
| ATOM | 238 | СВ | PHE | 29 | | 15.181 | 19.025 | 59.000 | | 14.20 |
| MOTA | 239 | CG | PHE | 29 | | 16.321 | 19.988 | 59.001 | 1.00 | 15.71 |
| ATOM | 240 | | PHE | 29 | | 17.354 | 19.871 | 58.075 | 1.00 | 14.27 |
| MOTA | 241 | CD2 | | 29 | | 16.371 | 21.008 | 59.946 | | 13.32 |
| MOTA | 242 | | PHE | 29 | | 18.423 | 20.764 | 58.080 | | 15.74 |
| ATOM | 243 | | PHE | 29 | | 17.430 | 21.904 | 59.967 | | 17.20 |
| ATOM | 244 | CZ | PHE | 29 | | 18.463 | 21.787 | 59.031 | | 14.83 |
| ATOM | 245 | С | PHE | 29 | | 14.044 | 17.284 | 60.383 | 1.00 | 15.83 |
| ATOM | 246 | Ō | PHE | 29 | | 13.481 | 17.696 | 61.398 | | 16.89 |
| ATOM | 247 | N | ALA | 30 | | 13.532 | 16.326 | 59.618 | | 16.16 |
| ATOM | 248 | CA | ALA | 30 | | 12.256 | 15.718 | 59.962 | | 17.31 |
| ATOM | 249 | CB | ALA | 30 | | 11.887 | 14.649 | 58.925 | | 16.54 |
| ATOM | 250 | C | ALA | 30 | | 12.343 | 15.094 | 61.357 | | 17.30 |
| ATOM | 251 | Ō | ALA | 30 | | 11.404 | 15.171 | 62.155 | | 16.42 |
| ATOM | 252 | N | LYS | 31 | | 13.481 | 14.467 | 61.634 | | 16.26 |
| ATOM | 253 | CA | LYS | 31 | | 13.731 | 13.815 | 62.918 | | 17.07 |
| ATOM | 254 | СВ | LYS | 31 | | 15.062 | 13.063 | 62.852 | | 18.24 |
| ATOM | 255 | CG | LYS | 31 | | 15.491 | 12.386 | 64.146 | | 24.20 |
| MOTA | 256 | CD | LYS | 31 | | 14.608 | 11.203 | 64.469 | | 27.80 |
| ATOM | 257 | CE | LYS | 31 | | 15.306 | 10.248 | 65.425 | | 30.36 |
| ATOM | 258 | NZ | LYS - | 31 | | 15.724 | 10.913 | 66.697 | | 32.82 |
| MOTA | 259 | С | LYS | 31 | | 13.788 | 14.833 | 64.057 | | 17.16 |
| | | | | | | | | | | |

| ATOM | 260 | 0 | LYS | 31 | 13.250 | 14.608 | 65.147 | 1.00 18.34 |
|--------------|------------|-----------|------------|----------|----------------|------------------|------------------|--------------------------|
| ATOM | 261 | N | LEU | 32 | 14.468 | 15.941 | 63.790 | 1.00 18.82 |
| ATOM | 262 | CA | LEU | 32 | 14.631 | 17.019 | 64.756 | 1.00 18.15 |
| ATOM | 263 | CB | LEU | 32 | 15.549 | 18.097 | 64.171 | 1.00 17.24 |
| MOTA | 264 | CG | LEU | 32 | 16.070 | 19.200 | 65.113 | 1.00 18.88 |
| MOTA | 265 | CD1 | LEU | 32 | 17.356 | 19.769 | 64.556 | 1.00 17.20 |
| MOTA | 266 | CD2 | LEU | 32 | 15.008 | 20.292 | 65.280 | 1.00 18.78 |
| MOTA | 267 | С | LEU | 32 | 13.272 | 17.620 | 65.103 | 1.00 18.02 |
| ATOM | 268 | 0 | LEU | 32 | 12.963 | 17.847 | 66.272 | 1.00 17.18 |
| ATOM | 269 | N | PHE | 33 | 12.462 | 17.885 | 64.083 | 1.00 17.34 |
| ATOM | 270 | CA | PHE | 33 | 11.144 | 18.473 | 64.316 | 1.00 18.21 |
| ATOM | 271 | CB | PHE | 33 | 10.451 | 18.832 | 62.995 | 1.00 15.31 |
| ATOM | 272 | CG | PHE | 33 | 11.255 | 19.734 | 62.092 | 1.00 14.93 |
| ATOM | 273 | CD1 | PHE | 33 | 12.133 | 20.689 | 62.610 | 1.00 14.65 |
| ATOM | 274 | CD2 | PHE | 33 | 11.093 | 19.657 | 60.716 | 1.00 13.00 |
| ATOM | 275 | CE1 | PHE | 33 | 12.832 | 21.550 | 61.764 | 1.00 13.96 |
| MOTA | 276 | CE2 | PHE | 33 | 11.783 | 20.510 | 59.861 | 1.00 9.75 |
| MOTA | 277 | CZ | PHE | 33 | 12.657 | 21.461 | 60.389 | 1.00 14.73 |
| MOTA | 278 | C | PHE | 33 | 10.255 | 17.503 | 65.091 | 1.00 18.11 |
| ATOM | 279 | 0 | PHE | 33 | 9.582 | 17.892 | 66.048 | 1.00 17.51 |
| MOTA | 280 | N | ALA | 34 | 10.246 | 16.241 | 64.666 | 1.00 18.42 |
| MOTA | 281 | CA | ALA | 34 | 9.433 | 15.231 | 65.330 | 1.00 19.46 |
| ATOM | 282 | CB | ALA | 34 | 9.573 | 13.878 | 64.623 | 1.00 20.93 |
| MOTA | 283 | С | ALA | 34 | 9.828 | 15.098 | 66.799 | 1.00 20.01 |
| MOTA | 284 | 0 | ALA | 34 | 8.970 | 15.000 | 67.673 | 1.00 19.41 |
| MOTA | 285 | N | ASP | 35 | 11.125 | 15.101 | 67.074 | 1.00 22.13 |
| MOTA | 286 | CA | ASP | 35 | 11.574 | 14.972 | 68.449 | 1.00 24.53 |
| MOTA | 287 | CB | ASP | 35 | 13.086 | 14.788 | 68.503 | 1.00 25.01 |
| MOTA | 288 | CG | ASP | 35 | 13.522 | 13.424 | 67.989 | 1.00 27.07 |
| MOTA | 289 | OD1 | ASP | 35 | 12.665 | 12.519 | 67.898 | 1.00 28.23 |
| MOTA | 290 | OD2 | ASP | 35 | 14.720 | 13.261 | 67.694 | 1.00 28.18 |
| MOTA | 291 | С | ASP | 35 | 11.156 | 16.151 | 69.324 | 1.00 23.50 |
| MOTA | 292 | 0 | ASP | 35 | 11.086 | 16.024 | 70.545 | 1.00 24.71 |
| MOTA | 293 | N | GLU | 36 | 10.872 | 17.294 | 68.706 | 1.00 24.53 |
| MOTA | 294 | CA | GLU | 36 | 10.455 | 18.469 | 69.464 | 1.00 23.98 |
| MOTA | 295 | CB | GLU | 36 | 11:029 | 19.743 | 68.841 | 1.00 25.45 |
| ATOM | 296 | CG | GLU | 36 | 12.535 | 19.876 | 68.963 | 1.00`25.52 |
| ATOM | 297 | CD | GLU | 36 | 13.005 | 19.750 | 70.399 | 1.00 26.66 |
| MOTA | 298 | | GLU | 36 | 12.385 | 20.375 | 71.286 | 1.00 23.68 |
| MOTA | 299 | | GLU | 36 | 13.993 | 19.032 | 70.637 | 1.00 27.91 |
| MOTA | 300 | С | GLU | 36 | 8.937 | 18.588 | 69.553 | 1.00 23.45 |
| MOTA | 301 | 0 | GLU | 36 | 8.421 | 19.502 | 70.192 | 1.00 23.61 |
| MOTA | 302 | N | GLY | 37 | 8.221 | 17.672 | 68.908 | 1.00 22.87 |
| MOTA | 303 | CA | GLY | 37 | 6.765 | 17.721 | 68.955 | 1.00 22.54 |
| ATOM | 304 | C | GLY | 37 | 6.096 | 18.447 | 67.796 | 1.00 19.79 |
| ATOM | 305 | O | GLY | 37 | 4.902 | 18.741 | 67.845 | 1.00 21.78 |
| MOTA | 306 | N | LEU | 38 | 6.873 | 18.755 | 66.765 | 1.00 19.44 |
| ATOM | 307 | CA | LEU | 38 | 6.365 | 19.416 | 65.569 | 1.00 19.71 |
| MOTA | 308 | CB | LEU | 38 | 7.459 | 20.281 | 64.952 | 1.00 20.11 |
| ATOM | 309 | CG | LEU | 38 | 7.131 | 21.691 | 64.458 | 1.00 22.03 |
| ATOM | 310 | | LEU | 38 | 8.352 | 22.238 | 63.739 | 1.00 20.65 |
| ATOM | 311 | | LEU | 38 | 5.918 | 21.714 | 63.548 | 1.00 20.80 |
| ATOM | 312 | C | LEU | 38 | 6.057 | 18.222 | 64.664 | 1.00 20.90 |
| ATOM | 313 | 0 | LEU | 38 | 6.938 | 17.741 | 63.939 | 1.00 18.42 |
| ATOM | 314 | N | ASN | 39 | 4.807 | 17.762 | 64.720 | 1.00 20.83 1.00 21.62 |
| ATOM | 315 | CA | ASN | 39 | 4.355 | 16.573 | 63.999 | |
| ATOM | 316 | CB | ASN | 39 | 3.489 4.128 | 15.709 15.480 | 64.924 66.281 | 1.00 24.31 1.00 28.12 |
| ATOM | 317 | CG OD1 | ASN | 39 | | | | 1.00 28.12 |
| ATOM | 318 319 | | ASN | 39 | 5.334 | 15.252 | 66.377 67.338 | 1.00 28.10 |
| ATOM | | | ASN | 39 | 3.321 | 15.526 | 62.696 | 1.00 29.42 |
| ATOM | 320 | C | ASN | 39 | 3.593 | 16.766 | | |
| ATOM | 321 | O | ASN | 39 | 2.955 3.648 | 15.832 17.961 | 62.221 62.123 | |
| ATOM | 322 | N | VAL | 40 | 2.960 | | | 1.00 19.39 |
| ATOM ATOM | 323 324 | CA CB | VAL VAL | 40 40 | 1.799 | 18.221 19.213 | 60.869 61.056 | 1.00 18.52 1.00 19.51 |
| | | | | | 1.113 | | | |
| ATOM ATOM | 325 326 | | VAL VAL | 40 40 | 0.801 | 19.470 18.659 | 59.726 62.066 | 1.00 18.68 1.00 18.86 |
| ATOM | 326 327 | CGZ | VAL · | 40 | 3.967 | 18.785 | 59.888 | 1.00 18.86 |
| ATOM | 328 | 0 | VAL | 40 | 4.450 | 19.910 | 60.040 | 1.00 18.22 |
| ATOM | 328 | Ŋ | MET | 41 | 4.450 | 17.990 | 58.869 | 1.00 14.68 |
| ATOM | 330 | CA | MET | 41 | 5.271 | 18.398 | 57.892 | 1.00 16.93 |
| ATOM | 331 | CB | MET | 41 | 6.535 | 17.556 | 58.082 | 1.00 16.29 |
| ATOM | 332 | CG | MET | 41 | 7.255 | 17.864 | 59.392 | 1.00 10.37 |
| ATOM | 333 | SD | MET | 41 | 8.564 | 16.706 | 59.719 | 1.00 20.16 |
| ATOM | 334 | CE | MET | 41 | 7.955 | 15.899 | 61.206 | 1.00 13.40 |
| ATOM | 335 | CE | MET | 41 | 4.804 | 18.342 | 56.452 | 1.00 21.43 |
| ATOM | 336 | 0 | MET | 41 | 4.046 | 17.464 | 56.062 | 1.00 18.81 |
| - | | - | | | | | | |

| ATOM | 337 | N | LEU | 42 | 5.276 | 19.300 | 55.665 | 1.00 18.90 |
|--------|-----|-----|------|------|--------|---------|--------|------------|
| ATOM | 338 | CA | LEU | 42 | 4.907 | 19.383 | 54.265 | 1.00 20.11 |
| ATOM | 339 | CB | LEU | 42 | 4.178 | 20.707 | 54.016 | 1.00 22.93 |
| ATOM | 340 | CG | LEU | 42 | 3.677 | 21.143 | 52.630 | 1.00 26.24 |
| ATOM | 341 | CD1 | LEU | 42 | 4.777 | 21.879 | 51.907 | 1.00 29.83 |
| ATOM | 342 | CD2 | LEU | 42 | 3.169 | 19.955 | 51.818 | 1.00 24.10 |
| MOTA | 343 | С | LEU | 42 | 6.120 | 19.258 | 53.344 | 1.00 19.47 |
| ATOM | 344 | 0 | LEU | 42 | 7.106 | 19.978 | 53.488 | 1.00 17.61 |
| ATOM | 345 | N | VAL | 43 | 6.045 | 18.313 | 52.414 | 1.00 19.14 |
| ATOM | 346 | CA | VAL | 43 | 7.102 | 18.116 | 51.429 | 1.00 18.25 |
| ATOM | 347 | CB | VAL | 43 | 7.332 | 16.624 | 51.126 | 1.00 19.90 |
| ATOM | 348 | | VAL | 43 | 8.397 | 16.461 | 50.041 | 1.00 19.97 |
| MOTA | 349 | CG2 | | 43 | 7.752 | 15.895 | 52.395 | 1.00 19.98 |
| ATOM | 350 | С | VAL | 43 | 6.517 | 18.806 | 50.208 | 1.00 18.93 |
| ATOM | 351 | 0 | VAL | 43 | 5.815 | 18.187 | 49.408 | 1.00 17.33 |
| ATOM | 352 | N | GLY | 44 | 6.786 | 20.102 | 50.089 | 1.00 17.93 |
| ATOM | 353 | CA | GLY | 44 | 6.248 | 20.865 | 48.980 | 1.00 20.04 |
| ATOM | 354 | С | GLY | 44 | 7.226 | 21.095 | 47.854 | 1.00 18.04 |
| ATOM | 355 | 0 | GLY | 44 | 8.430 | 20.872 | 48.008 | 1.00 17.40 |
| ATOM | 356 | N | ASP | 45 | 6.715 | 21.557 | 46.718 | 1.00 18.65 |
| ATOM | 357 | CA | ASP | 45 | 7.583 | 21.796 | 45.575 | 1.00 20.74 |
| ATOM | 358 | СВ | ASP | 45 | 6.764 | 21.936 | 44.279 | 1.00 21.58 |
| ATOM | 359 | CG | ASP | 45 | 5.684 | 22.997 | 44.372 | 1.00 23.34 |
| ATOM | 360 | OD1 | ASP | 45 | 5.672 | 23.751 | 45.359 | 1.00 22.56 |
| ATOM | 361 | OD2 | ASP | 45 | 4.858 | 23.074 | 43.442 | 1.00 21.88 |
| ATOM | 362 | С | ASP | 45 | 8.483 | 23.007 | 45.776 | 1.00 19.43 |
| ATOM | 363 | 0 | ASP | 45 | 9.243 | 23.374 | 44.883 | 1.00 19.95 |
| ATOM | 364 | N | SER | 46 | 8.408 | 23.635 | 46.949 | 1.00 20.64 |
| ATOM | 365 | CA | SER | 46 | 9.285 | 24.772 | 47.211 | 1.00 19.31 |
| ATOM | 366 | CB | SER | 46 | 8.944 | 25.429 | 48.551 | 1.00 19.58 |
| ATOM | 367 | OG | SER | 46 | 9.146 | 24.533 | 49.628 | 1.00 20.11 |
| ATOM | 368 | С | SER | 46 | 10.705 | 24.206 | 47.243 | 1.00 19.27 |
| ATOM | 369 | 0 | SER | 46 | 11.686 | 24.945 | 47.155 | 1.00 20.36 |
| ATOM | 370 | N | LEU | 47 | 10.810 | 22.884 | 47.365 | 1.00 18.59 |
| ATOM | 371 | CA | LEU | 47 | 12.119 | 22.237 | 47.384 | 1.00 19.25 |
| ATOM ' | 372 | CB | LEU | 47 | 11.970 | 20.737 | 47.661 | 1.00 18.00 |
| ATOM | 373 | ÇG | LEU | 47 | 11.308 | 19.853 | 46.597 | 1.00 17.40 |
| ATOM | 374 | CD1 | LEU | 47 | 12.309 | 19.517 | 45.489 | 1.00 15.15 |
| ATOM | 375 | CD2 | LEU | 47 | 10.822 | 18.572 | 47.255 | 1.00 16.79 |
| MOTA | 376 | С | LEU | 47 | 12.853 | 22.467 | 46.063 | 1.00 17.82 |
| ATOM | 377 | 0 | LEU | 47 | 14.083 | 22.399 | 46.004 | 1.00 17.99 |
| ATOM | 378 | N | GLY | 48 | 12.100 | 22.742 | 45.001 | 1.00 17.81 |
| ATOM | 379 | CA | GLY | 48 | 12.720 | 22.997 | 43.708 | 1.00 16.18 |
| ATOM | 380 | С | GLY | 48 | 13.659 | 24.186 | 43.784 | 1.00 18.66 |
| ATOM | 381 | 0 | GLY | 48 | 14.644 | 24.271 | 43.050 | 1.00 17.89 |
| ATOM | 382 | N | MET | 49 | 13.356 | 25.108 | 44.691 | 1.00 19.84 |
| ATOM | 383 | CA | MET | 49 | 14.172 | 26.303 | 44.865 | 1.00 20.69 |
| ATOM | 384 | CB | MET | 49 | 13.263 | 27.515 | 45.100 | 1.00 23.46 |
| ATOM | 385 | CG | MET' | 49 | 12.312 | 27.789 | 43.940 | 1.00 25.97 |
| ATOM | 386 | SD | MET | 49 | 11.099 | 29.069 | 44.266 | 1.00 31.34 |
| ATOM | 387 | CE | MET | 49 | 12.037 | 3.0.520 | 43.900 | 1.00 32.33 |
| MOTA | 388 | C | MET | 49 | 15.162 | 26.153 | 46.022 | 1.00 20.49 |
| MOTA | 389 | O | MET | 49 | 16.370 | 26.292 | 45.837 | 1.00 22.08 |
| ATOM | 390 | N | THR | 50 | 14.649 | 25.846 | 47.208 | 1.00 21.41 |
| ATOM | 391 | CA | THR | 50 | 15.492 | 25.702 | 48.387 | 1.00 21.56 |
| ATOM | 392 | CB | THR | 50 | 14.636 | 25.608 | 49.655 | 1.00 25.24 |
| MOTA | 393 | OG1 | THR | 50 | 15.493 | 25.523 | 50.801 | 1.00 31.31 |
| ATOM | 394 | | THR | 50 | 13.750 | 24.381 | 49.600 | 1.00 23:80 |
| ATOM | 395 | С | THR | 50 | 16.432 | 24.498 | 48.362 | 1.00 21.30 |
| MOTA | 396 | 0 | THR | 50 | 17.551 | 24.565 | 48.864 | 1.00 21.10 |
| ATOM | 397 | N | VAL | 51 | 15.975 | 23.391 | 47.787 | 1.00 18.20 |
| MOTA | 398 | CA | VAL | 51 | 16.812 | 22.200 | 47.719 | 1.00 19.81 |
| ATOM | 399 | CB | VAL | 51 | 15.997 | 20.918 | 47.983 | 1.00 18.02 |
| MOTA | 400 | CG1 | | 51 | 16.909 | 19.695 | 47.900 | 1.00 23.01 |
| ATOM | 401 | | VAL | 51 | 15.355 | 20.983 | 49.365 | 1.00 21.92 |
| ATOM | 402 | C | VAL | 51 | 17.536 | 22.038 | 46.384 | 1.00 18.45 |
| ATOM | 403 | 0 | VAL | 51 | 18.755 | 21.867 | 46:351 | 1.00 16.95 |
| MOTA | 404 | N | GLN | 52 | 16.788 | 22.087 | 45.286 | 1.00 17.92 |
| ATOM | 405 | CA | GLN | 52 | 17.381 | 21.907 | 43.963 | 1.00 18.16 |
| MOTA | 406 | CB | GLN | 52 | 16.312 | 21.427 | 42.976 | 1.00 17.32 |
| ATOM | 407 | CG | GLN | 52 | 15.529 | 20.227 | 43.482 | 1.00 16.59 |
| ATOM | 408 | CD | GLN | 52 | 14.477 | 19.771 | 42.504 | 1.00 15.57 |
| MOTA | 409 | | GLN | 52 | 14.011 | 20.552 | 41.673 | 1.00 16.27 |
| ATOM | 410 | | GLN | 52 | 14.084 | 18.504 | 42.600 | 1.00 14.83 |
| MOTA | 411 | C | GLN | 52 | 18.076 | 23.150 | 43.411 | 1.00 18.00 |
| MOTA | 412 | 0 | GLN | . 52 | 19.003 | 23.052 | 42.606 | 1.00 18.07 |
| ATOM | 413 | N | GLY | 53 | 17.624 | 24.324 | 43.831 | 1.00 19.93 |

| MOTA | 414 | CA | GLY | 53 | 18.248 | 25.549 | 43.361 | 1.00 20.83 |
|--------|------------|--------|------------|----------|--------|--------|--------|------------|
| ATOM | 415 | C | GLY | 53 | 17.685 | 26.146 | 42.085 | 1.00 22.32 |
| ATOM | 416 | 0 | GLY | 53 | 18.387 | 26.877 | 41.387 | 1.00 24.49 |
| MOTA | 417 | N | HIS | 54 | 16.429 | 25.849 | 41.771 | 1.00 22.93 |
| ATOM | 418 | CA | HIS | 54 | 15.803 | 26.397 | 40.575 | 1.00 24.27 |
| ATOM | 419 | CB | HIS | 54 | 14.725 | 25.438 | 40.049 | 1.00 23.64 |
| MOTA | 420 | CG | HIS | 54 | 15.264 | 24.127 | 39.568 | 1.00 25.03 |
| | | | | 54 | 15.030 | | 39.984 | 1.00 25.03 |
| MOTA | 421 | CD2 | | | | 22.860 | | |
| MOTA | 422 | ND1 | | 54 | 16.175 | 24.029 | 38.538 | 1.00 25.82 |
| MOTA | 423 | CE1 | | 54 | 16.481 | 22.759 | 38.343 | 1.00 26.94 |
| MOTA | 424 | NE2 | | 54 | 15.800 | 22.029 | 39.208 | 1.00 26.01 |
| MOTA | 425 | C | HIS | 54 | 15.176 | 27.748 | 40.914 | 1.00 25.18 |
| MOTA | 426 | 0 | HIS | 54 | 14.947 | 28.058 | 42.086 | 1.00 24.14 |
| ATOM | 427 | N | ASP | 55 | 14.898 | 28.545 | 39.884 | 1.00 25.82 |
| ATOM | 428 | CA | ASP | 55 | 14.302 | 29.869 | 40.062 | 1.00 27.59 |
| MOTA | 429 | CB | ASP | 55 | 14.550 | 30.729 | 38.813 | 1.00 30.40 |
| MOTA | 430 | CG | ASP | 55 | 13.786 | 30.232 | 37.600 | 1.00 33.05 |
| ATOM | 431 | OD1 | | 55 | 12.535 | 30.266 | 37.622 | 1.00 36.66 |
| ATOM | 432 | OD2 | | 55 | 14.428 | 29.804 | 36.618 | 1.00 37.40 |
| ATOM | 433 | C | ASP | 55 | 12.801 | 29.778 | 40.333 | 1.00 26.78 |
| ATOM | 434 | ō | ASP | 55 | 12.174 | 30.755 | 40.737 | 1.00 27.57 |
| | 435 | N | SER | 56 | 12.228 | 28.600 | 40.099 | 1.00 25.17 |
| ATOM | | | | 56 | 10.802 | 28.386 | 40.322 | 1.00 23.17 |
| ATOM | 436 | CA | SER | | | | | |
| ATOM | 437 | CB | SER | 56 | 10.008 | 28.635 | 39.036 | 1.00 21.35 |
| ATOM | 438 | OG | SER | 56 | 10.232 | 27.608 | 38.084 | 1.00 21.31 |
| MOTA | 439 | С | SER | 56 | 10.582 | 26.956 | 40.795 | 1.00 20.02 |
| ATOM | 440 | 0 | SER | 56 | 11.529 | 26.177 | 40.903 | 1.00 21.16 |
| ATOM | 441 | N | THR | 57 | 9.334 | 26.615 | 41.084 | 1.00 19.01 |
| ATOM · | 442 | CA | THR | 57 | 9.007 | 25.272 | 41.543 | 1.00 19.21 |
| ATOM | 443 | CB | THR | 57 | 7.869 | 25.305 | 42.579 | 1.00 19.53 |
| ATOM | 444 | OG1 | THR | 57 | 6.686 | 25.840 | 41.972 | 1.00 20.97 |
| ATOM | 445 | CG2 | THR | 57 | 8.249 | 26.179 | 43.772 | 1.00 19.07 |
| ATOM | 446 | С | THR | 57 | 8.560 | 24.359 | 40.396 | 1.00 18.44 |
| ATOM | 447 | 0 | THR | 57 | 8.422 | 23.153 | 40.587 | 1.00 18.34 |
| ATOM | 448 | N | LEU . | 58 | 8.341 | 24.930 | 39.212 | 1.00 20.59 |
| ATOM | 449 | CA | LEU | 58 | 7.868 | 24.149 | 38.062 | 1.00 20.34 |
| ATOM | 450 | CB | LEU | 58 | 7.720 | 25.029 | 36.816 | 1.00 20.92 |
| | 451 | CG | LEU | 58 | 6.542 | 26.005 | 36.785 | 1.00 23.24 |
| MOTA | | | | | | 27.242 | 37.578 | 1.00 25.30 |
| ATOM | 452 | CD1 | | 58 | 6.926 | | | |
| MOTA | 453 | CD2 | | 58 | 6.195 | 26.393 | 35.349 | |
| MOTA | 454 | С | LEU | 58 | 8.687 | 22.913 | 37.696 | 1.00 21.07 |
| MOTA | 455 | 0 | LEU | 58 | 8.120 | 21.868 | 37.366 | 1.00 19.23 |
| ATOM | 456 | N | PRO | 59 | 10.025 | 23.015 | 37.731 | 1.00 20.10 |
| ATOM | 457 | CD | PRO | 59 | 10.845 | 24.213 | 37.965 | 1.00 23.05 |
| ATOM | 458 | CA | PRO | 59 | 10.862 | 21.860 | 37.392 | 1.00 21.47 |
| ATOM | 459 | CB | PRO | 59 | 12.286 | 22.433 | 37.427 | 1.00 21.53 |
| ATOM | 460 | CG | PRO | 59 | 12.167 | 23.617 | 38.335 | 1.00 25.99 |
| ATOM | 461 | С | PRO | 59 | 10.678 | 20.653 | 38.307 | 1.00 18.05 |
| MOTA | 462 | 0 | PRO | 59 | 11.041 | 19.534 | 37.946 | 1.00 18.36 |
| ATOM | 463 | N | VAL | 60 | 10.100 | 20.865 | 39.486 | 1.00 17.05 |
| | 464 | CA | VAL | 60 | 9.882 | 19.760 | 40.423 | 1.00 16.87 |
| ATOM | 465 | СВ | VAL | 60 | 9.330 | 20.273 | 41.785 | 1.00 15.81 |
| ATOM | 466 | | VAL | 60 | 9.046 | 19.099 | 42.709 | 1.00 15.77 |
| ATOM | 467 | CG2 | VAL | 60 | 10.336 | 21.201 | 42.438 | 1.00 15.49 |
| | | | | | 8.894 | 18.740 | 39.852 | 1.00 13.43 |
| ATOM | 468 | С 0 | VAL | 60 | 7.805 | 19.099 | 39.406 | 1.00 17.80 |
| ATOM | 469 470 | | VAL THR | 60 61 | 9.267 | 17.465 | 39.406 | 1.00 18.90 |
| ATOM | | N | | | | | | |
| ATOM | 471 | CA | THR | 61 | 8.389 | 16.420 | 39.352 | 1.00 20.57 |
| ATOM | 472 | CB | THR | 61 | 9.124 | 15.590 | 38.252 | 1.00 24.68 |
| MOTA | 473 | OG1 | THR | 61 | 9.451 | 16.440 | 37.146 | 1.00 30.75 |
| MOTA | 474 | CG2 | THR | 61 | 8.261 | 14.425 | 37.760 | 1.00 30.08 |
| ATOM | 475 | С | THR | 61 | 7.906 | 15.507 | 40.487 | 1.00 17.77 |
| ATOM | 476 | 0 | THR | 61 | 8.408 | 15.581 | 41.606 | 1.00 16.02 |
| MOTA | 477 | N | VAL | 62 | 6.919 | 14.662 | 40.196 | 1.00 15.87 |
| MOTA | 478 | CA | VAL | 62 | 6.360 | 13.734 | 41.177 | 1.00 15.01 |
| ATOM | 479 | СВ | VAL | 62 | 5.269 | 12.834 | 40.532 | 1.00 13.13 |
| ATOM | 480 | CG1 | VAL | 62 | 4.831 | 11.742 | 41.512 | 1.00 13.60 |
| ATOM | 481 | CG2 | VAL | 62 | 4.070 | 13.696 | 40.116 | 1.00 13.51 |
| ATOM | 482 | C | VAL | 62 | 7.428 | 12.837 | 41.784 | 1.00 15.22 |
| ATOM | 483 | ō | VAL | 62 | 7.390 | 12.529 | 42.978 | 1.00 16.66 |
| ATOM | 484 | N | ALA | 63 | 8.383 | 12.412 | 40.965 | 1.00 15.74 |
| ATOM | 485 | CA | ALA | 63 | 9.445 | 11.551 | 41.467 | 1.00 14.86 |
| ATOM | 486 | CB | ALA | 63 | 10.383 | 11.137 | 40.319 | 1.00 16.20 |
| | | | | | 10.333 | 12.264 | 42.562 | 1.00 13.05 |
| ATOM | 487 | C . | ALA | 63 | | | 43.573 | |
| ATOM | 488 | 0 | ALA | 63 | 10.579 | 11.655 | | 1.00 13.87 |
| MOTA | 489 | N | ASP | 64 | 10.505 | 13.551 | 42.363 | 1.00 14.03 |
| ATOM | 490 | CA | ASP | 64 | 11.258 | 14.319 | 43.357 | 1.00 14.19 |
| | | | | | | | | |

| ATOM | 491 | CB | ASP | 64 | 11.507 | 15.762 | 42.890 | 1.00 13.98 |
|--------------|------------|-----|------------|----------|------------------|------------------------------|------------------|--------------------------|
| ATOM | 492 | CG | ASP | 64 | 12.309 | 15.849 | 41.605 | 1.00 14.58 |
| ATOM | 493 | | ASP | 64 | 13.170 | 14.975 | 41.351 | 1.00 15.44 |
| АТОМ | 494 | | ASP | 64 | 12.093 | 16.829 | 40.846 | 1.00 17.47 |
| ATOM | 495 | С | ASP | 64 | 10.492 | 14.355 | 44.679 | 1.00 14.42 |
| ATOM | 496 | 0 | ASP | 64 | 11.072 | 14.125 | 45.740 | 1.00 12.00 |
| ATOM | 497 | N | ILE | 65 | 9.194 | 14.649 | 44.618 | 1.00 13.48 |
| ATOM | 498 | CA | ILE | 65 | 8.374 | 14.705 | 45.827 | 1.00 13.80 |
| ATOM | 499 | CB | ILE | 65 | 6.899 | 15.082 | 45.504 | 1.00 11.05 |
| ATOM | 500 | CG2 | | 65 | 6.042 | 14.958 | 46.773 | 1.00 13.85 |
| ATOM | 501 | | ILE | 65 | 6.822 | 16.488 | 44.929 | 1.00 14.20 |
| ATOM | 502 | CD1 | | 65 | 7.176 | 17.602 | 45.914 | 1.00 13.32 |
| MOTA | 503 | С | ILE | 65 | 8.382 | 13.359 | 46.551 | 1.00 12.47 |
| ATOM | 504 | 0 | ILE | 65 | 8.502 | 13.294 | 47.769 | 1.00 13.03 |
| ATOM | 505 | N | ALA | 66 | 8.252 | 12.279 | 45.786 | 1.00 12.41 |
| ATOM | 506 | CA | ALA | 66 | 8.217 | 10.933 | 46.356 | 1.00 9.78 |
| MOTA | 507 | CB | ALA | 66 | 7.938 | 9.913 | 45.252 | 1.00 9.59 |
| ATOM | 508 | С | ALA | 66 | 9.518 | 10.582 | 47.077 | 1.00 11.07 |
| ATOM | 509 | 0 | ALA | 66 | 9.529 | 9.899 | 48.103 | 1.00 11.14 |
| ATOM | 510 | N | TYR | 67 | 10.619 | 11.023 | 46.492 | 1.00 11.42 |
| MOTA | 511 | CA | TYR | 67 | 11.944 | 10.790 | 47.048 | 1.00 12.07 |
| MOTA | 512 | CB | TYR | 67 | 12.977 | 11.335 | 46.061 | 1.00 11.65 |
| MOTA | 513 | CG | TYR | 67 | 14.394 | 11.327 | 46.566 | 1.00 13.46 |
| ATOM | 514 | CD1 | TYR | 67 | 15.120 | 10.146 | 46.641 | 1.00 13.65 |
| MOTA | 515 | CE1 | TYR | 67 | 16.441 | 10.144 | 47.081 | 1.00 15.17 |
| MOTA | 516 | CD2 | TYR | 67 | 15.018 | 12.515 | 46.949 | 1.00 16.34 |
| MOTA | 517 | CE2 | TYR | 67 | 16.333 | 12.529 | 47.389 | 1.00 13.50 |
| MOTA | 518 | CZ | TYR | 67 | 17.039 | 11.340 | 47.451 | 1.00 16.29 |
| MOTA | 519 | OH | TYR | 67 | 18.351 | 11.348 | 47.874 | 1.00 16.32 |
| MOTA | 520 | С | TYR | 67 | 12.082 | 11.487 | 48.414 | 1.00 12.63 |
| MOTA | 521 | 0 | TYR | 67 | 12.501 | 10.878 | 49.406 | 1.00 12.25 |
| MOTA | 522 | N | HIS | 68 | 11.713 | 12.765 | 48.455 | 1.00 14.09 |
| MOTA | 523 | CA | HIS | 68 | 11.814 | 13.548 | 49.688 | 1.00 13.34 |
| ATOM | 524 | CB | HIS | 68 | 11.723 | 15.039 | 49.358 | 1.00 12.95 |
| MOTA | 525 | CG | HIS | 68 | 12.930 | 15.561 | 48.644 | 1.00 13.09 |
| ATOM | 526 | | HIS | 68 | 13.146 | 15.833 | 47.335 | 1.00 13.59 |
| ATOM | 527 | | HIS | 68 | 14.128 | 15.794 | 49.285 | 1.00 11.39 |
| MOTA | 528 | | HIS | 68 | 15.030 | 16.185 | 48.403 | 1.00 13.50 |
| ATOM | 529 | NE2 | | 68 | 14.461 | 16.217 | 47.211 | 1.00 14.36 |
| ATOM | 530 | С | HIS | 68 | 10.771 | 13.147 | 50.722 | 1.00 14.18 |
| ATOM | 531 | 0 | HIS | 68 | 11.002 | 13.282 | 51.929 | 1.00 12.96 |
| MOTA | 532 | N | THR | 69 | 9.631 | 12.651 | 50.247 | 1.00 13.76 |
| ATOM | 533 | CA | THR | 69 | 8.572 | 12.193 | 51.125 | 1.00 12.86 |
| ATOM | 534 | CB | THR | 69 | 7.291 | 11.816 | 50.321 | 1.00 13.67 |
| ATOM | 535 | | THR | 69 | 6.692 | 13.004 | 49.794 | 1.00 13.10 |
| ATOM | 536 | | THR | 69 | 6.290 | 11.098 | 51.200 | 1.00 13.21 |
| ATOM | 537 | С | THR | 69 | 9.080 | 10.957 | 51.877 | 1.00 12.94 |
| ATOM | 538 | 0 | THR | 69 | 8.891 | 10.837 | 53.086 51.166 | 1.00 13.96 1.00 12.91 |
| ATOM | 539 | N | ALA | 70 | 9.736 10.266 | 10.045 _. 8.840 | 51.795 | 1.00 12.91 |
| ATOM | 540 541 | CA | ALA | 70 70 | | 7.924 | 50.743 | 1.00 12.83 |
| MOTA | | CB | ALA | 70 70 | 10.905 | 9.166 | 52.893 | 1.00 13.23 |
| ATOM | 542 | С | ALA ALA | 70 70 | 11.285 11.278 | 8.543 | 53.959 | 1.00 13.23 |
| ATOM ATOM | 543 544 | Ŋ | ALA | 71 | 12.157 | 10.136 | 52.635 | 1.00 12.50 |
| ATOM | 545 | CA | ALA | 71 | 13.174 | 10.519 | 53.613 | 1.00 13.30 |
| ATOM | 546 | CB | ALA | 71 | 14.166 | 11.480 | 52.984 | 1.00 14.53 |
| ATOM | 547 | C | ALA | 71 | 12.539 | 11.153 | 54.845 | 1.00 14.10 |
| ATOM | 548 | Ö. | ALA | 71 | 12.935 | 10.876 | 55.981 | 1.00 14.47 |
| ATOM | 549 | N | VAL | 72 | 11.542 | 11.999 | 54.622 | 1.00 14.55 |
| ATOM | 550 | CA | VAL | 72 | 10.861 | 12.654 | 55.736 | 1.00 15.46 |
| ATOM | 551 | CB | VAL | 72 | 9.830 | 13.682 | 55.227 | 1.00 16.14 |
| ATOM | 552 | | VAL · | 72 | 9.000 | 14.217 | 56.394 | 1.00 16.03 |
| ATOM | 553 | | VAL | 72 | 10.540 | 14.808 | 54.509 | 1.00 16.34 |
| ATOM | 554 | c | VAL | 72 | 10.153 | 11.606 | 56.590 | 1.00 15.16 |
| ATOM | 555 | Õ | VAL | 72 | 10.183 | | 57.824 | 1.00 14.69 |
| ATOM | 556 | N | ARG | 73 | 9.522 | 10.633 | 55.936 | 1.00 14.57 |
| ATOM | 557 | CA | ARG | 73 | 8.815 | 9.593 | 56.669 | 1.00 12.67 |
| ATOM | 558 | CB | ARG | 73 | 8.060 | 8.654 | 55.719 | 1.00 13.42 |
| ATOM | 559 | CG | ARG | 73 | 7.356 | 7.508 | 56.447 | 1.00 12.53 |
| ATOM | 560 | CD | ARG | 73 | 6.380 | 8.015 | 57.520 | 1.00 16.45 |
| MOTA | 561 | NE | ARG | 73 | 5.237 | 8.713 | 56.933 | 1.00 16.27 |
| ATOM | 562 | CZ | ARG | 73 | 4.358 | 9.437 | 57.617 | 1.00 17.72 |
| MOTA | 563 | NH1 | | 73 | 4.479 | 9.573 | 58.934 | 1.00 13.94 |
| MOTA | 564 | NH2 | ARG | 73 | 3.353 | 10.027 | 56.982 | 1.00 16.25 |
| MOTA | 565 | С | ARG | 73 | 9.748 | 8.767 | 57.540 | 1.00 12.87 |
| MOTA | 566 | 0 | ARG | 73 | 9.369 | | 58.631 | 1.00 13.64 |
| ATOM | 567 | N | ARG | 74 | 10.963 | 8.524 | 57.057 | 1.00 14.65 |

| ATOM | 568 | CA | ARG | 74 | 11.926 | 7.738 | 57.823 | 1.00 13.53 |
|--------|------|------|-------|----------|--------|-------------|--------|------------|
| ATOM | 569 | CB | ARG | 74 | 13.155 | 7.405 | 56.975 | 1.00 15.28 |
| ATOM | 570 | CG | ARG | 74 | 12.860 | 6.543 | 55.752 | 1.00 16.51 |
| ATOM | 571 | CD | ARG | 74 | 14.133 | 5.937 | 55.155 | 1.00 17.73 |
| ATOM | 572 | NE | ARG | 74 | 13.895 | 5.341 | 53.838 | 1.00 20.82 |
| ATOM | 573 | CZ | ARG | 74 | 13.896 | 6.020 | 52.694 | 1.00 22.35 |
| ATOM | 574 | | ARG | 74 | 14.127 | 7.325 | 52.688 | 1.00 23.90 |
| ATOM | 575 | | ARG | 74 | 13.656 | 5.397 | 51.552 | 1.00 27.63 |
| ATOM | 576 | C | ARG | 74 | 12.355 | 8.513 | 59.052 | 1.00 16.13 |
| ATOM | 577 | ō | ARG | 74 | 12.673 | 7.932 | 60.093 | 1.00 16.86 |
| | 578 | N | GLY | 75 | 12.359 | 9.834 | 58.923 | 1.00 16.62 |
| ATOM | | | | 75 75 | 12.753 | 10.681 | 60.035 | 1.00 10.62 |
| ATOM | 579 | CA | GLY | | | | | |
| ATOM | 580 | C | GLY . | 75 75 | 11.629 | 10.935 | 61.019 | 1.00 17.81 |
| MOTA | 581 | 0 | GLY | 75 | 11.865 | 11.107 | 62.215 | 1.00 17.98 |
| MOTA | 582 | N | ALA | 76 | 10.398 | 10.952 | 60.525 | 1.00 17.56 |
| MOTA | 583 | CA | ALA | 76 | 9.240 | 11.210 | 61.385 | 1.00 17.19 |
| MOTA | 584 | CB | ALA | 76 | 8.767 | 12.640 | 61.173 | 1.00 16.95 |
| MOTA | 585 | С | ALA | 76 | 8.108 | 10.229 | 61.094 | 1.00 18.56 |
| ATOM | 586 | 0 | ALA | 76 | 7.100 | 10.590 | 60.492 | 1.00 18.58 |
| ATOM | 587 | N | PRO | 77 | 8.255 | 8.976 | 61.549 | 1.00 20.24 |
| ATOM | 588 | CD | PRO | 77 | 9.361 | 8.507 | 62.400 | 1.00 21.81 |
| MOTA | 589 | CA | PRO | 77 | 7.271 | 7.908 | 61.348 | 1.00 20.91 |
| ATOM | 590 | CB | PRO | 77 | 7.949 | 6.698 | 61.982 | 1.00 22.03 |
| ATOM | 591 | CG | PRO | 77 | 8.749 | 7.303 | 63.072 | 1.00 25.30 |
| ATOM | 592 | С | PRO | 77 | 5.870 | 8.138 | 61.902 | 1.00 20.81 |
| MOTA | 593 | 0 | PRO | 77 | 4.929 | 7.462 | 61.488 | 1.00 20.60 |
| MOTA | 594 | N | ASN | 78 | 5.720 | 9.080 | 62.828 | 1.00 19.26 |
| MOTA | 595 | CA | ASN | 78 | 4.402 | 9.342 | 63.399 | 1.00 20.69 |
| ATOM | 596 | CB | ASN | 78 | 4.449 | 9.242 | 64.932 | 1.00 22.75 |
| ATOM | 597 | CG | ASN | 78 | 4.554 | 7.806 | 65.414 | 1.00 27.00 |
| ATOM | 598 | OD1 | ASN | 78 | 3.772 | 6.951 | 65.001 | 1.00 31.16 |
| ATOM | 599 | ND2 | | 78 | 5.515 | 7.534 | 66.287 | 1.00 29.98 |
| ATOM | 600- | С | ASN | 78 | 3.821 | 10.693 | | 1.00 19.38 |
| MOTA | 601 | 0 | ASN | 78 | 2.750 | 11.076 | 63.456 | 1.00 21.43 |
| ATOM | 602 | N | CYS | 79 | 4.507 | 11.399 | 62.104 | 1.00 17.77 |
| ATOM | 603 | CA | CYS | 79 | 4.040 | 12.713 | 61.686 | 1.00 19.13 |
| ATOM | 604 | СВ | CYS | 79 | 5.210 | 13.553 | 61.150 | 1.00 19.79 |
| ATOM | 605 | SG | CYS | 79 | 5.646 | 13.275 | 59.389 | 1.00 24.05 |
| ATOM | 606 | C | CYS | 79 | 2.938 | 12.667 | 60.633 | 1.00 19.96 |
| ATOM | 607 | 0 | CYS | 79 | 2.735 | 11.652 | 59.961 | 1.00 17.94 |
| ATOM | 608 | N | LEU | 80 | 2.202 | 13.770 | 60.528 | 1.00 17.54 |
| | 609 | CA | | 80 | 1.163 | 13.770 | 59.519 | 1.00 19.33 |
| ATOM | | | LEU | | | | | |
| ATOM | 610 | CB | LEU | 80 | 0.054 | 14.860 | 59.978 | 1.00 20.96 |
| MOTA | 611 | CG | LEU | 80 | -0.984 | 15.225 | 58.909 | 1.00 21.27 |
| ATOM | 612 | CD1 | | 80 | -1.670 | 13.967 | 58.396 | 1.00 22.20 |
| ATOM | 613 | CD2 | LEU | 80 | -2.008 | 16.195 | 59.488 | 1.00 22.16 |
| ATOM | 614 | С | LEU | 80 | 1.962 | 14.527 | 58.387 | 1.00 18.90 |
| ATOM | 615 | 0 | LEU | 80 | 2.442 | 15.655 | 58.509 | 1.00 18.11 |
| ATOM | 616 | N | LEU | 81 | 2.120 | 13.788 | 57.294 | 1.00 15.94 |
| MOTA | 617 | CA | LEU | 81 | 2.924 | 14.261 | 56.181 | 1.00 16.28 |
| MOTA | 618 | CB | LEU | 81 | 3.930 | 13.169 | 55.775 | 1.00 18.46 |
| ATOM | 619 | CG | LEU | 81 | 5.213 | 13.532 | 55.008 | 1.00 18.26 |
| ATOM | 620 | CD1 | | 81 | 6.102 | 12.304 | 54.937 | 1.00 18.48 |
| ATOM | 621 | CD2 | | 81 | 4.884 | 14.038 | 53.605 | 1.00 21.41 |
| MOTA | 622 | С | LEU | 81 | 2.090 | 14.669 | 54.986 | 1.00 16.06 |
| ATOM | 623 | 0 | LEU | 81 | 1.357 | 13.857 | 54.417 | 1.00 16.48 |
| ATOM | 624 | Ν . | LEU | 82 | 2.183 | 15.944 | 54.628 | 1.00 16.31 |
| ATOM | 625 | CA | LEU | 82 | 1.457 | 16.466 | 53.477 | 1.00 17.30 |
| MOTA | 626 | CB | LEU | 82 | 0.897 | 17.859 | 53.766 | 1.00 19.25 |
| ATOM | 627 | CG · | LEU | 82 | -0.451 | 17.985 | 54.495 | 1.00 22.19 |
| ATOM · | 628 | CD1 | | 82 | -0.449 | 17.200 | 55.792 | 1.00 21.32 |
| MOTA | 629 | CD2 | LEU | 82 | -0.720 | 19.462 | 54.750 | 1.00 21.16 |
| ATOM | 630 | C. | LEU | 82 | 2.458 | 16.557 | 52.342 | 1.00 17.89 |
| MOTA | 631 | 0 | LEU | 82 | 3.560 | 17.068 | 52.531 | 1.00 18.88 |
| MOTA | 632 | N | ALA | 83 | 2.092 | 16.053 | 51.171 | 1.00 16.82 |
| MOTA | 633 | CA | ALA | 83 | 2.997 | 16.114 | 50.033 | 1.00 16.39 |
| MOTA | 634 | CB | ALA | 83 . | 3.406 | 14.720 | 49.607 | 1.00 16.49 |
| ATOM | 635 | С | ALA | 83 | 2.337 | 16.841 | 48.881 | 1.00 14.35 |
| ATOM | 636 | 0 | ALA | 83 | 1.186 | 16.579 | 48.554 | 1.00 14.15 |
| ATOM | 637 | N | ASP | 84 | 3.058 | 17.775 | 48.274 | 1.00 13.95 |
| ATOM | 638 | CA | ASP | 84 | 2.498 | 18.505 | 47.148 | 1.00 16.00 |
| ATOM | 639 | СВ | ASP | 84 | 3.268 | 19.799 | 46.893 | 1.00 22.80 |
| ATOM | 640 | CG | ASP | 84 | 2.767 | 20.957 | 47.723 | 1.00 24.54 |
| ATOM | 641 | OD1 | | 84 | 1.548 | 21.195 | 47.752 | 1.00 30.38 |
| ATOM | 642 | | ASP | 84 | 3.602 | 21.644 | 48.329 | 1.00 32.60 |
| ATOM | 643 | C | ASP | 84 | 2.526 | 17.716 | 45.851 | 1.00 16.16 |
| ATOM | 644 | ō | ASP | 84 | 3.400 | 16.875 | 45.640 | 1.00 14.13 |
| | _ | - | | | | · · · · · · | | |

| ATOM | 645 | N | LEU | 85 | 1.535 | 17.967 | 44.998 | 1.00 15.10 |
|-------|-----|-----|-----|----|---------|--------|--------|------------|
| ATOM | 646 | CA | LEU | 85 | 1.539 | 17.381 | 43.667 | 1.00 15.19 |
| ATOM | 647 | СВ | LEU | 85 | 0.127 | 17.043 | 43.167 | 1.00 16.96 |
| ATOM | 648 | CG | LEU | 85 | -0.451 | 15.751 | 43.751 | 1.00 17.98 |
| | 649 | CD1 | | 85 | -1.753 | 15.360 | 43.028 | 1.00 17.36 |
| ATOM | | | | | | | | |
| ATOM | 650 | CD2 | LEU | 85 | 0.574 | 14.639 | 43.604 | 1.00 17.58 |
| ATOM | 651 | C | LEU | 85 | 2.111 | 18.593 | 42.937 | 1.00 14.95 |
| MOTA | 652 | 0 | LEU | 85 | 1.563 | 19.694 | 43.024 | 1.00 15.92 |
| ATOM | 653 | N | PRO | 86 | 3.255 | 18.419 | 42.262 | 1.00 14.05 |
| MOTA | 654 | CD | PRO | 86 | 3.984 | 17.143 | 42.170 | 1.00 15.98 |
| MOTA | 655 | CA | PRO | 86 | 3.949 | 19.473 | 41.518 | 1.00 15.84 |
| MOTA | 656 | CB | PRO | 86 | 5.306 | 18.839 | 41.224 | 1.00 16.60 |
| ATOM | 657 | CG | PRO | 86 | 4.933 | 17.386 | 41.018 | 1.00 16.94 |
| MOTA | 658 | С | PRO | 86 | 3.249 | 19.970 | 40.255 | 1.00 17.90 |
| ATOM | 659 | Ο. | PRO | 86 | 2.161 | 19.515 | 39.899 | 1.00 17.49 |
| ATOM | 660 | N | PHE | 87 | 3.897 | 20.917 | 39.591 | 1.00 17.02 |
| ATOM | 661 | CA | PHE | 87 | 3.386 | 21.509 | 38.371 | 1.00 18.00 |
| ATOM | 662 | CB | PHE | 87 | 4.486 | 22.357 | 37.728 | 1.00 19.87 |
| ATOM | 663 | CG | PHE | 87 | 4.125 | 22.906 | 36.383 | 1.00 19.63 |
| ATOM | 664 | | PHE | 87 | 3.025 | 23.739 | 36.229 | 1.00 19.99 |
| MOTA | 665 | | PHE | 87 | 4.893 | 22.588 | 35.265 | 1.00 20.71 |
| MOTA | 666 | | PHE | 87 | 2.692 | 24.249 | 34.982 | 1.00 21.55 |
| | | CE2 | PHE | | 4.567 | | | 1.00 21.33 |
| MOTA | 667 | | | 87 | | 23.095 | 34.012 | |
| ATOM | 668 | CZ | PHE | 87 | 3.466 | 23.926 | 33.870 | 1.00 21.84 |
| ATOM | 669 | С | PHE | 87 | 2.871 | 20.467 | 37.373 | 1.00 17.52 |
| MOTA | 670 | O | PHE | 87 | 3.561 | 19.495 | 37.051 | 1.00 16.53 |
| MOTA | 671 | N | MET | 88 | 1.644 | 20.682 | 36.909 | 1.00 16.65 |
| ATOM | 672 | CA | MET | 88 | 0.984 | 19.816 | 35.936 | 1.00 18.63 |
| MOTA | 673 | CB | MET | 88 | 1.666 | 19.944 | 34.575 | 1.00 20.77 |
| MOTA | 674 | CG | MET | 88 | 0.767 | 19.578 | 33.413 | 1.00 22.54 |
| MOTA | 675 | SD | MET | 88 | -0.593 | 20.732 | 33.216 | 1.00 21.14 |
| MOTA | 676 | CE | MET | 88 | 0.111 | 21.920 | 32.099 | 1.00 22.91 |
| ATOM | 677 | С | MET | 88 | 0.931. | 18.340 | 36.326 | 1.00 19.33 |
| ATOM | 678 | ō | MET | 88 | 0.987 | 17.463 | 35.461 | 1.00 22.28 |
| ATOM | 679 | N | ALA | 89 | 0.822 | 18.062 | 37.619 | 1.00 17.87 |
| ATOM | 680 | CA | ALA | 89 | 0.749 | 16.685 | 38.086 | 1.00 17.24 |
| ATOM | 681 | CB | ALA | 89 | 1.609 | 16.506 | 39.333 | 1.00 17.24 |
| ATOM | 682 | C | ALA | | -0.701 | 16.285 | 38.379 | 1.00 16.47 |
| ATOM | 683 | | ALA | 89 | -0.701 | 15.164 | 38.816 | 1.00 10.30 |
| | | 0 | | | | | 38.145 | 1.00 17.43 |
| ATOM | 684 | N | TYR | 90 | -1.624 | 17.209 | | |
| ATOM | 685 | CA | TYR | 90 | -3.041 | 16.942 | 38.364 | 1.00 15.59 |
| ATOM | 686 | CB | TYR | 90 | -3.452 | 17.350 | 39.790 | 1.00 14.88 |
| MOTA | 687 | CG | TYR | 90 | -2.959 | 18.715 | 40.223 | 1.00 15.60 |
| MOTA | 688 | CD1 | TYR | 90 | -3.753 | 19.854 | 40.064 | 1.00 17.89 |
| MOTA | 689 | | TYR | 90 | -3.288 | 21.117 | 40.454 | 1.00 17.95 |
| ATOM | 690 | CD2 | TYR | 90 | -1.690 | 18.870 | 40.782 | 1.00 17.54 |
| MOTA | 691 | CE2 | TYR | 90 | -1.217 | 20.122 | 41.173 | 1.00 17.49 |
| ATOM | 692 | CZ | TYR | 90 | -2.016 | 21.235 | 41.008 | 1.00 18.23 |
| MOTA | 693 | OH | TYR | 90 | -1.543 | 22.470 | 41.404 | 1.00 19.18 |
| ATOM | 694 | С | TYR | 90 | -3.885 | 17.666 | 37.322 | 1.00 15.82 |
| ATOM | 695 | Ο΄ | TYR | 90 | -4.937 | 18.225 | 37.628 | 1.00 17.20 |
| ATOM | 696 | N | ALA | 91 | -3.412 | 17.628 | 36.079 | 1.00 16.74 |
| MOTA | 697 | CA | ALA | 91 | -4.085 | 18.272 | 34.959 | 1.00 17.95 |
| ATOM | 698 | CB | ALA | 91 | -3.177 | 18.262 | 33.731 | 1.00 18.19 |
| ATOM | 699 | C | ALA | 91 | -5.425 | 17.611 | 34.631 | 1.00 17.59 |
| ATOM | 700 | ō | ALA | 91 | -6.289 | 18.230 | 34.010 | 1.00 16.62 |
| ATOM | 701 | N | THR | 92 | -5.580 | 16.347 | 35.015 | 1.00 16.91 |
| ATOM | 701 | CA | THR | 92 | -6.838 | 15.619 | 34.811 | 1.00 15.64 |
| ATOM | 703 | CB | THR | 92 | -6.821 | 14.689 | 33.566 | 1.00 17.31 |
| | | OG1 | | 92 | -5.942 | 13.582 | 33.804 | 1.00 17.31 |
| ATOM | 704 | | THR | | -6.369 | | 32.322 | 1.00 15.98 |
| ATOM | 705 | CG2 | THR | 92 | | 15.438 | 36.021 | |
| ATOM | 706 | C | THR | 92 | -7.052 | 14.720 | | |
| ATOM | 707 | 0 | THR | 92 | -6.097 | 14.366 | 36.711 | 1.00 17.07 |
| ATOM | 708 | N | PRO | 93 | -8.310 | 14.339 | 36.299 | 1.00 16.42 |
| ATOM | 709 | CD | PRO | 93 | -9.570 | 14.771 | 35.669 | 1.00 17.40 |
| ATOM | 710 | CA | PRO | 93 | -8.568 | 13.470 | 37.447 | 1.00 15.13 |
| ATOM | 711 | CB | PRO | 93 | -10.056 | 13.168 | 37.312 | 1.00 17.06 |
| MOTA | 712 | CG | PRO | 93 | -10.589 | 14.464 | 36.750 | 1.00 16.77 |
| MOTA | 713 | С | PRO | 93 | -7.696 | 12.210 | 37.411 | 1.00 16.09 |
| MOTA | 714 | 0 | PRO | 93 | -7.028 | 11.879 | 38.396 | 1,00 13.79 |
| MOTA | 715 | N | GLU | 94 | -7.689 | 11.517 | 36.273 | 1.00 16.39 |
| MOTA | 716 | CA | GLU | 94 | -6.882 | 10.305 | 36.120 | 1.00 17.29 |
| MOTA | 717 | CB | GLU | 94 | -6.948 | 9.791 | 34.680 | 1.00 20.57 |
| MOTA | 718 | CG | GLU | 94 | -8.040 | 8.779 | 34.426 | 1.00 27.03 |
| ATOM | 719 | CD | GLU | 94 | -7.968 | 8.209 | 33.024 | 1.00 30.80 |
| MOTA | 720 | | GLU | 94 | -6.908 | 7.660 | 32.659 | 1.00 34.96 |
| ATOM- | 721 | | GLU | 94 | -8.965 | 8.309 | 32.285 | 1.00 36.52 |
| | | | | | | | | |

| ATOM | 722 | С | GLU | 94 | -5.418 | 10.492 | 36.497 | 1.00 17.89 |
|------|------------|-----|----------------------|-----|----------|--------|--------|------------|
| ATOM | 723 | 0 | GLU | 94 | -4.846 | 9.658 | 37.194 | 1.00 16.77 |
| ATOM | 724 | N | GLN | 95 | -4.806 | 11.573 | 36.029 | 1.00 15.83 |
| ATOM | 725 | CA | GLN | 95 | -3.408 | 11.811 | 36.350 | 1.00 16.28 |
| ATOM | 726 | CB | GLN | 95 | -2.845 | 12.932 | 35.491 | 1.00 18.34 |
| | | | | 95 | -2.936 | 12.662 | 34.002 | 1.00 24.91 |
| ATOM | 727 | CG | GLN | | | | | |
| ATOM | 728 | CD | GLN | 95 | -2.424 | 13.826 | 33.189 | 1.00 29.82 |
| ATOM | 729 | OE1 | | 95 | -1.215 | 14.043 | 33.081 | 1.00 31.53 |
| MOTA | 730 | NE2 | | 95 | -3.347 | 14.606 | 32.632 | 1.00 31.62 |
| MOTA | 731 | C | GLN | 95 | -3.232 | 12.144 | 37.817 | 1.00 13.83 |
| MOTA | 732 | 0 | GLN | 95 | -2.245 | 11.743 | 38.422 | 1.00 14.18 |
| ATOM | 733 | N | ALA | 96 | -4.173 | 12.888 | 38.393 | 1.00 12.99 |
| ATOM | 734 | CA | ALA | 96 | -4.071 | 13.213 | 39.813 | 1.00 11.89 |
| ATOM | 735 | CB | ALA | 96 | -5.229 | 14.113 | 40.243 | 1.00 10.87 |
| ATOM | 736 | C | ALA | 96 | -4.090 | 11.911 | 40.611 | 1.00 12.60 |
| ATOM | 737 | ō | ALA | 96 | -3.311 | 11.746 | 41.549 | 1.00 11.80 |
| ATOM | 738 | N | PHE | 97 | -4.970 | 10.979 | 40.236 | 1.00 12.82 |
| | | | | | | | 40.256 | 1.00 12.02 |
| ATOM | 739 | CA | PHE | 97 | -5.050 | 9.709 | | |
| ATOM | 740 | CB | PHE | 97 | -6.072 | 8.741 | 40.332 | 1.00 13.33 |
| MOTA | 741 | CG | PHE | 97 | -7.459 | 9.303 | 40.173 | 1.00 14.06 |
| ATOM | 742 | | PHE | 97 | -7.975 | 10.220 | 41.079 | 1.00 14.07 |
| ATOM | 743 | CD2 | PHE | 97 | -8.254 | 8.891 | 39.113 | 1.00 13.38 |
| MOTA | 744 | CE1 | PHE | 97 | -9.273 | 10.725 | 40.931 | 1.00 11.22 |
| ATOM | 745 | CE2 | PHE | 97 | -9.556 | 9.385 | 38.948 | 1.00 13.40 |
| ATOM | 746 | CZ | PHE | 97 | -10.061 | 10.302 | 39.859 | 1.00 11.20 |
| MOTA | 747 | C | PHE | 97 | -3.699 | 8.990 | 40.975 | 1.00 13.62 |
| ATOM | 748 | ō | PHE | 97 | -3.244 | 8.552 | 42.026 | 1.00 13.09 |
| ATOM | 749 | N | GLU | 98 | -3.064 | 8.856 | 39.815 | 1.00 14.92 |
| ATOM | 750 | CA | GLU | 98 | -1.786 | 8.154 | 39.768 | 1.00 14.32 |
| | | | | | | | 38.327 | 1.00 10.75 |
| ATOM | 751 | CB | GLU | 98 | -1.356 | 7.859 | | |
| ATOM | 752 | CG | GLU | 98 | -0.045 | 7.064 | 38.268 | 1.00 28.53 |
| MOTA | 753 | CD | GLU | 98 | -0.113 | 5.768 | 39.066 | 1.00 33.54 |
| ATOM | 754 | OE1 | | 98 | -0.767 | 4.810 | 38.587 | 1.00 35.57 |
| MOTA | -755 | OE2 | GLU | 98 | 0.472 | 5.706 | 40.187 | 1.00 34.76 |
| MOTA | 756 | С | GLU | 98 | -0.660 | 8.888 | 40.480 | 1.00 14.28 |
| MOTA | 757 | 0 | GLU | 98 | 0.134 | 8.275 | 41.198 | 1.00 14.65 |
| ATOM | 758 | N | ASN | 99 | -0.580 | 10.196 | 40.294 | 1.00 12.45 |
| MOTA | 759 | CA | ASN | 99 | 0.490 | 10.944 | 40.941 | 1.00 11.69 |
| ATOM | 760 | CB | ASN | 99 | 0.627 | 12.329 | 40.299 | 1.00 11.89 |
| ATOM | 761 | CG | ASN | 99 | 1.172 | 12.238 | 38.890 | 1.00 12.59 |
| ATOM | 762 | | ASN | 99 | 2.019 | 11.384 | 38.609 | 1.00 13.02 |
| ATOM | 763 | ND2 | | 99 | 0.707 | 13.105 | 38.002 | 1.00 13.56 |
| | | | | 99 | 0.707 | | 42.451 | |
| MOTA | 764 | C | ASN | | | 11.026 | | |
| ATOM | | 0 | ASN | 99 | 1.256 | 10.953 | 43.216 | 1.00 11.87 |
| MOTA | 766 | N | ALA | 100 | -0.970 | 11.157 | 42.879 | 1.00 12.15 |
| ATOM | 767 | CA | ALA | 100 | -1.284 | 11.189 | 44.306 | 1.00 14.14 |
| MOŢA | 768 | CB | ALA | 100 | -2.777 | 11.489 | 44.531 | 1.00 13.05 |
| ATOM | 769 | С | ALA | 100 | -0.940 | 9.814 | 44.878 | 1.00 12.60 |
| ATOM | 770 | 0 | ALA | 100 | -0.347 | 9.709 | 45.953 | 1.00 13.66 |
| ATOM | 771 | N | ALA | 101 | -1.312 | 8.748 | 44.175 | 1.00 12.06 |
| ATOM | 772 | CA | ALA | 101 | -0.999 | 7.412 | 44.679 | 1.00 10.87 |
| ATOM | 773 | СВ | ALA | 101 | -1.590 | 6.338 | 43,755 | 1.00 10.90 |
| ATOM | 774 | c | ALA | 101 | 0.517 | 7.204 | 44.853 | 1.00 10.31 |
| ATOM | 775 | ō | ALA | 101 | 0.953 | 6.543 | 45.794 | 1.00 12.24 |
| ATOM | 776 | N | THR | 102 | 1.322 | 7.766 | 43.754 | 1.00 12.24 |
| | | | | | 2.781 | 7.606 | 44.046 | 1.00 10.77 |
| ATOM | 777 770 | CA | THR | 102 | | | | |
| MOTA | 778 | CB | THR | 102 | 3.450 | 8.244 | 42.833 | 1.00 11.82 |
| ATOM | 779 | OG1 | | 102 | 3.011 | 7.556 | 41.648 | 1.00 12.54 |
| MOTA | 780 | CG2 | | 102 | 4.965 | 8.143 | 42.934 | 1.00 13.14 |
| MOTA | 781 | C · | THR | 102 | 3.329 | 8.218 | 45.331 | 1.00 12.67 |
| MOTA | 782 | 0 | THR | 102 | 4.122 | 7.609 | 46.053 | 1.00 13.26 |
| MOTA | 783 | N | VAL | 103 | 2.872 | 9.430 | 45.608 | 1.00 13.06 |
| MOTA | 784 | CA | VAL | 103 | 3.275 | 10.178 | 46.786 | 1.00 17.15 |
| MOTA | 785 | СВ | VAL | 103 | 2.771 | 11.622 | 46.644 | 1.00 20.15 |
| ATOM | 786 | | VAL | 103 | 2.563 | 12.250 | 47.990 | 1.00 26.49 |
| ATOM | 787 | | VAL | 103 | 3.758 | 12.408 | 45.807 | 1.00 21.10 |
| ATOM | 788 | C | VAL | 103 | 2.769 | 9.533 | 48.084 | 1.00 16.61 |
| ATOM | 789 | 0 | VAL | 103 | 3.477 | 9.519 | 49.097 | 1.00 14.86 |
| | | | | | | | | |
| ATOM | 790 | N | MET | 104 | 1.554 | 8.989 | 48.048 | 1.00 13.98 |
| ATOM | 791 | CA | MET | 104 | 0.976 | 8.336 | 49.219 | 1.00 13.90 |
| ATOM | 792 | CB | MET | 104 | -0.514 | 8.053 | 48.997 | 1.00 16.23 |
| MOTA | 793 | CG | MET | 104 | -1.373 | 9.288 | 48.838 | 1.00 20.48 |
| MOTA | 794 | SD | MET | 104 | -1.516 | 10.232 | 50.350 | 1.00 23.82 |
| MOTA | 795 | CE | MET | 104 | ' -2.587 | 9.130 | 51.315 | 1.00 23.65 |
| MOTA | 796 | С | MET | 104 | 1.701 | 7.031 | 49.537 | 1.00 13.22 |
| MOTA | 797 | 0 | MET | 104 | 1.979 | 6.735 | 50.707 | 1.00 13.56 |
| | | | | 105 | 2.008 | 6.242 | 48.508 | 1.00 13.42 |
| ATOM | 798 | N | ARG | 103 | 2 | | | |

| ATOM | 799 | CA | ARG | 105 | | 2.711 | 4.989 | 48.743 | 1.00 11.59 |
|--------------|--------------|--------------|------------|------------|---|------------------|------------------|------------------|--------------------------|
| ATOM | 800 | CB | ARG | 105 | | 2.817 | 4.152 | 47.453 | 1.00 14.28 |
| ATOM | 801 | CG | ARG | 105 | | 1.492 | 3.637 | 46.914 | 1.00 15.18 |
| MOTA | 802 | CD | ARG | 105 | | 1.673 | 2.542 | 45.848 | 1.00 15.37 |
| ATOM | 803 | NE | ARG | 105 | | 0.436 | 2.355 | 45.086 | 1.00 18.07 |
| MOTA | 804 805 | CZ NILI 1 | ARG ARG | 105 105 | | 0.151 1.021 | 2.986 3.837 | 43.951 43.420 | 1.00 16.17 1.00 14.58 |
| ATOM ATOM | 806 | | ARG | 105 | | -1.030 | 2.802 | 43.420 | 1.00 14.38 |
| ATOM | 807 | C | ARG | 105 | | 4.112 | 5.296 | 49.275 | 1.00 10.65 |
| ATOM | 808 | Ō | ARG | 105 | | 4.684 | 4.494 | 50.009 | 1.00 12.75 |
| MOTA | 809 | N | ALA | 106 | | 4.645 | 6.463 | 48.916 | 1.00 12.09 |
| ATOM | 810 | CA | ALA | 106 | | 5.978 | 6.873 | 49.346 | 1.00 13.06 |
| ATOM | 811 | CB | ALA | 106 | | 6.496 | 7.999 | 48.455 | 1.00 14.76 |
| ATOM | 812 | C | ALA | 106 | | 6.015 | 7.305 | 50.807 | 1.00 15.39 |
| ATOM ATOM | 813 814 | O N | ALA GLY | 106 107 | | 7.094 4.841 | 7.529 7.430 | 51.365 51.420 | 1.00 15.17 1.00 14.50 |
| ATOM | 815 | CA | GLY | 107 | | 4.779 | 7.806 | 52.821 | 1.00 14.87 |
| ATOM | 816 | C | GLY | 107 | | 3.904 | 8.991 | 53.207 | 1.00 15.59 |
| MOTA | 817 | 0 | GLY | 107 | | 3.751 | 9.273 | 54.393 | 1.00 16.79 |
| MOTA | 818 | N | | 108 | | 3.331 | 9.691 | 52.238 | 1.00 13.12 |
| MOTA | 819 | CA | ALA | 108 | | 2.484 | 10.833 | 52.569 | 1.00 13.97 |
| ATOM | 820 | CB | ALA | 108 | | 2.307 | 11.724 | 51.342 | 1.00 14.04 1.00 14.46 |
| ATOM ATOM | 821 822 | C O | ALA ALA | 108 108 | | 1.122 0.696 | 10.374 9.251 | 53.099 52.834 | 1.00 14.46 1.00 14.12 |
| ATOM | 823 | N | ASN | 109 | | 0.461 | 11.230 | 53.880 | 1.00 14.94 |
| ATOM | 824 | CA | ASN | 109 | | -0.863 | 10.919 | 54.440 | 1.00 14.90 |
| MOTA | 825 | CB | ASN | 109 | | -0.947 | 11.277 | 55.931 | 1.00 14.17 |
| MOTA | 826 | CG | ASN | 109 | | 0.012 | 10.493 | 56.790 | 1.00 14.97 |
| MOTA | 827 | OD1 | | 109 | | -0.101 | 9.276 | 56.926 | 1.00 16.84 |
| ATOM | 828 | | ASN | 109 | | 0.959 | 11.193 | 57.388 | 1.00 14.33 |
| ATOM ATOM | 829 830 | С О | ASN ASN | 109 109 | | -1.901 -3.102 | 11.781 11.556 | 53.737 53.870 | 1.00 13.58 1.00 15.82 |
| ATOM | 831 | N | MET | 110 | | -1.427 | 12.768 | 52.991 | 1.00 13.52 |
| ATOM | 832 | CA | MET | 110 | | -2.316 | 13.704 | 52.332 | 1.00 14.31 |
| MOTA | 833 | CB | MET | 110 | • | -2.828 | 14.688 | 53.394 | 1.00 14.27 |
| MOTA | 834 | CG | MET | 110 | | -3.595 | 15.902 | 52.910 | 1.00 19.21 |
| MOTA | 835 | SD | MET | 110 | | -4.143 | 16.871 | 54.371 | 1.00 20.75 |
| ATOM ATOM | 836 837 . | CE C | MET MET | 110 110 | | -5.845 -1.576 | 16.364 14.431 | 54.495 51.219 | 1.00 18.93 1.00 13.50 |
| ATOM | 838 | 0 | MET | 110 | | -0.358 | 14.635 | 51.219 | 1.00 13.30 |
| ATOM | 839 | N | VAL | 111 | | -2.323 | 14.810 | 50.191 | 1.00 13.28 |
| MOTA | 840 | CA | VAL | 111 | | -1.765 | 15.507 | 49.050 | 1.00 15.44 |
| MOTA | 841 | СВ | VAL | 111 | | -2.175 | 14.786 | 47.752 | 1.00 18.91 |
| MOTA | 842 | CG1 | | 111 | | -1.800 -1.504 | 15.614 | 46.564 47.691 | 1.00 21.41 1.00 16.70 |
| ATOM ATOM | 843 844 | CG2 C | VAL VAL | 111 111 | | -2.271 | 13.416 16.944 | 49.000 | 1.00 15.70 |
| ATOM | 845 | ō | VAL | 111 | | -3.420 | 17.209 | 49.344 | 1.00 16.27 |
| MOTA | 846 | N | LYS | 112 | | -1.411 | 17.869 | 48.586 | 1.00 18.00 |
| ATOM | 847 | CA | LYS | 112 | | -1.810 | 19.266 | 48.475 | 1.00 17.62 |
| ATOM | 848 | CB | LYS | 112 | | -0.912 | 20.174 | 49.324 | 1.00 16.94 1.00 18.28 |
| ATOM | 849 850 | CG | LYS | 112 112 | | -1.299 -0.768 | 21.650 22.491 | 49.203 50.354 | 1.00 18.28 1.00 20.19 |
| ATOM | 851 | CE | LYS | 112 | | 0.738 | 22.675 | 50.334 | 1.00 20.13 |
| MOTA | 852 | NZ | LYS | 112 | | 1.171 | 23.485 | 49.116 | 1.00 22.77 |
| ATOM | 853 | С | LYS | 112 | | -1.738 | 19.707 | 47.022 | 1.00 18.52 |
| ATOM | 854 | 0 | LYS | 112 | | -0.741 | 19.461 | 46.330 | 1.00 18.26 |
| ATOM ATOM | 855 856 | N CA | ILE ILE | 113 113 | | -2.800 -2.878 | 20.360 20.836 | 46.563 45.187 | 1.00 18.70 1.00 19.67 |
| MOTA | 857 | СВ | ILE | 113 | | -3.852 | 19.967 | 44.359 | 1.00 20.73 |
| | 858 | CG2 | ILE | 113 | | -3.270 | 18.573 | 44.169 | 1.00 20.69 |
| MOTA | 859 | CG1 | ILE | 113 | | -5.201 | 19.870 | 45.067 | 1.00 21.18 |
| MOTA | 860 | CD1 | | 113 | | -6.238 | 19.041 | 44.316 | 1.00 22.35 |
| MOTA ATOM | 861 862 | С 0 | ILE ILE | 113 113 | | -3.349 -4.206 | 22.288 22.694 | 45.139 45.919 | 1.00 20.68 1.00 23.09 |
| ATOM | 863 | N | GLU | 114 | | -2.775 | 23.055 | 44.217 | 1.00 20.92 |
| MOTA | 864 | CA | GLU | 114 | | -3.094 | 24.468 | 44.041 | 1.00 22.18 |
| MOTA | 865 | CB | GLU | 114 | | -1.872 | 25.219 | 43.510 | 1.00 23.81 |
| ATOM | 866 | CG | GLU | 114 | | -0.715 | 25.328 | 44.478 | 1.00 25.94 |
| MOTA MOTA | 867 868 | CD OE1 | GLU | 114 114 | | 0.474 0.296 | 26.052 26.741 | 43.872 42.844 | 1.00 27.17 1.00 28.77 |
| ATOM | 869 | OE2 | GLU | 114 | | 1.588 | 25.947 | 44.427 | 1.00 29.32 |
| MOTA | 870 | C | GLU | 114 | | -4.247 | 24.707 | 43.074 | 1.00 23.10 |
| ATOM | 871 | 0 | GLU | 114 | | -4.325 | 24.072 | 42.025 | 1.00 22.98 |
| ATOM | 872 | N | GLY | 115 | | -5.135 | 25.636 | 43.420 | 1.00 22.55 |
| MOTA MOTA | 873 874 | CA C | GLY GLY | 115 115 | | -6.246 -7.581 | 25.933 26.079 | 42.534 43.230 | 1.00 24.88 1.00 24.82 |
| ATOM | 875 | 0 | GLY | 115 | | -7.720 | 25.743 | 44.406 | 1.00 24.02 |

| ATOM | 876 | N | GLY | 116 | -8.569 | 26.582 | 42.496 | 1.00 25.06 |
|--------------|--------------|--------|-----|-----|--------------------|--------|--------|--------------------------|
| ATOM | 877 | CA | GLY | 116 | -9.889 | 26.767 | 43.066 | 1.00 25.41 |
| ATOM | 878 | C | GLY | 116 | -10.964 | 25.864 | 42.490 | 1.00 26.85 |
| ATOM | 879 | ō | GLY | 116 | -10.767 | 24.659 | 42.346 | 1.00 26.53 |
| | 880 | N | GLU | 117 | -12.105 | 26.468 | 42.166 | 1.00 26.32 |
| ATOM | | | | | | • | | |
| MOTA | 881 | CA | GLU | 117 | -13.268 | 25.782 | 41.606 | 1.00 27.23 |
| MOTA | 882 | CB | GLU | 117 | -14.205 | 26.810 | 40.959 | 1.00 31.55 |
| MOTA | 883 | CG | GLU | 117 | -15.191 | 27.444 | 41.923 | 1.00 36.76 |
| MOTA | 884 | CD | GLU | 117 | -16.448 | 26.615 | 42.091 | 1.00 40.05 |
| MOTA | 885 | OE1 | GLU | 117 | -16.341 | 25.369 | 42.112 | 1.00 39.80 |
| MOTA | 886 | OE2 | GLU | 117 | -17.543 | 27.210 | 42.211 | 1.00 41.02 |
| ATOM | 887 | С | GLU | 117 | -13.021 | 24.661 | 40.602 | 1.00 24.91 |
| ATOM | 888 | 0 | GLU | 117 | -13.621 | 23.592 | 40.715 | 1.00 24.23 |
| ATOM | 889 | N | TRP | 118 | -12.155 | 24.904 | 39.622 | 1.00 23.95 |
| ATOM | 890 | CA | TRP | 118 | -11.880 | 23.906 | 38.588 | 1.00 23.05 |
| ATOM | 891 | CB | TRP | 118 | -10.853 | 24.437 | 37.574 | 1.00 22.93 |
| MOTA | 892 | CG | TRP | 118 | -9.417 | 24.433 | 38.027 | 1.00 22.06 |
| ATOM | 893 | CD2 | TRP | 118 | -8.430 | 23.432 | 37.736 | 1.00 22.29 |
| ATOM | 894 | CE2 | TRP | 118 | -7.227 | 23.836 | 38.356 | 1.00 21.75 |
| ATOM | 895 | CE3 | TRP | 118 | -8.449 | 22.231 | 37.015 | 1.00 21.59 |
| ATOM | 896 | | | 118 | -8.787 | 25.377 | 38.790 | 1.00 22.77 |
| ATOM | 897 | NE1 | TRP | 118 | -7.472 | 25.027 | 38.989 | 1.00 23.97 |
| ATOM | 898 | CZ2 | TRP | 118 | -6.049 | 23.082 | 38.272 | 1.00 21.19 |
| ATOM | 899 | CZ3 | TRP | 118 | -7.273 | 21.478 | 36.932 | 1.00 19.76 |
| ATOM | 900 | CH2 | TRP | 118 | -6.093 | 21.908 | 37.558 | 1.00 13.70 |
| MOTA | 901 | C | TRP | 118 | -11.415 | 22.562 | 39.137 | 1.00 10.03 |
| | | | | | -11.413 | | | |
| ATOM | 902 | 0 | TRP | 118 | -10.933 | 21.542 | 38.453 | 1.00 22.61 |
| ATOM | 903 | N | LEU | 119 | | 22.563 | 40.375 | 1.00 22.53 |
| ATOM | 904 | CA | LEU | 119 | -10.445 | 21.343 | 41.017 | 1.00 21.12 |
| MOTA | 905 | CB | LEU | 119 | -9.323 | 21.686 | 42.000 | 1.00 22.00 |
| MOTA | 906 | CG | LEU | 119 | -7.951 | 21.956 | 41.397 | 1.00 22.79 |
| ATOM | 907 | | LEU | 119 | -6.976 | 22.370 | 42.489 | 1.00 23.33 |
| MOTA | 908 | | LEU | 119 | -7.469 | 20.690 | 40.691 | 1.00 24.30 |
| MOTA | 909 | C | LEU | 119 | -11.502 | 20.541 | 41.759 | 1.00 20.72 |
| MOTA | 910 | 0 | LEU | 119 | -11.232 | 19.422 | 42.193 | 1.00 21.92 |
| MOTA | 911 | N | VAL | 120 | -12.699 | 21.101 | 41.908 | 1.00 19.20 |
| MOTA | 912 | CA | VAL | 120 | -13.766 | 20.419 | 42.638 | 1.00 19.95 |
| MOTA | 913 | CB | VAL | 120 | -15.127 | 21.122 | 42.429 | 1.00 22.03 |
| MOTA | 914 | CG1 | VAL | 120 | -16.258 | 20.225 | 42.907 | 1.00 24.11 |
| ATOM | 915 | CG2 | VAL | 120 | -15.150 | 22.429 | 43.201 | 1.00 25.29 |
| ATOM | 916 | C | VAL | 120 | -13.921 | 18.940 | 42.301 | 1.00 18.47 |
| MOTA | 917 | 0 | VAL | 120 | -13.961 | 18.093 | 43.196 | 1.00 16.89 |
| ATOM | 918 | N | GLU | 121 | -14.004 | 18.624 | 41.015 | 1.00 17.81 |
| ATOM | 919 | CA | GLU | 121 | -14.163 | 17.237 | 40.611 | 1.00 17.82 |
| ATOM | 920 | CB | GLU | 121 | -14.344 | 17.150 | 39.094 | 1.00 21.67 |
| MOTA | 921 | CG | GLU | 121 | -14.418 | 15.728 | 38.576 | 1.00 25.89 |
| ATOM | 922 | CD | GLU | 121 | -14.824 | 15.658 | 37.114 | 1.00.31.46 |
| ATOM | 923 | | GLU | 121 | -14.246 | 16.399 | 36.290 | 1.00 33.28 |
| ATOM | 924 | OE2 | | 121 | -15.717 | 14.848 | 36.793 | 1.00 33.12 |
| ATOM | 925 | C | GLU | 121 | -12.977 | 16.385 | 41.057 | 1.00 16.63 |
| ATOM | 926 | ō | GLU | 121 | -13.153 | 15.288 | 41.592 | 1.00 15.69 |
| ATOM | 927 | N | THR | 122 | -11.772 | 16.901 | 40.846 | 1.00 16.55 |
| ATOM | 928 | CA | THR | 122 | -10.557 | 16.188 | 41.230 | 1.00 15.50 |
| ATOM | 929 | CB | THR | 122 | -9.291 | 17.010 | 40.858 | 1.00 16.20 |
| ATOM | 930 | OG1 | THR | 122 | -9.292 | 17.251 | 39.447 | 1.00 18.56 |
| ATOM | 931 | CG2 | | 122 | -8.009 | 16.250 | 41.215 | 1.00 15.78 |
| ATOM | 932 | C | | 122 | -10.571 | 15.891 | 42.729 | 1.00 15.78 |
| | | | THR | | | | | |
| ATOM ATOM | 933 934 | O N | THR | 122 | -10.300 -10.905 | 14.769 | 43.145 | 1.00 14.26 1.00 16.07 |
| | | N | VAL | 123 | | 16.890 | 43.539 | |
| ATOM | 935 | CA | VAL | 123 | -10.942 | 16.691 | 44.982 | 1.00 15.30 |
| MOTA | 936 | CB | VAL | 123 | -11.265 | 17.993 | 45.722 | 1.00 16.32 |
| ATOM | 937 | CG1 | | 123 | -11.382 | 17.733 | 47.217 | 1.00 15.84 |
| MOTA | 938 | CG2 | | 123 | -10.194 | 19.023 | 45.431 | 1.00 17.06 |
| ATOM | 939 | C | VAL | 123 | -11.964 | 15.649 | 45.392 | 1.00 16.79 |
| ATOM | 940 | О | VAL | 123 | -11.685 | 14.793 | 46.237 | 1.00 13.71 |
| ATOM | 941 | N | GLN | 124 | -13.155 | 15.728 | 44.803 | 1.00 15.90 |
| MOTA | 942 | CA | GLN | 124 | -14.227 | 14.790 | 45.122 | 1.00 17.82 |
| MOTA | 943 | CB | GLN | 124 | -15.498 | 15.146 | 44.333 | 1.00 19.74 |
| MOTA | 944 | ÇG | GLN | 124 | -16.018 | 16.566 | 44.586 | 1.00 27.73 |
| MOTA | 945 | CD | GLN | 124 | -17.335 | 16.871 | 43.871 | 1.00 30.08 |
| ATOM | 946 | OE1 | GLN | 124 | -17.414 | 16.825 | 42.641 | 1.00 33.03 |
| MOTA | 947 | NE2 | GLN | 124 | -18.370 | 17.190 | 44.643 | 1.00 28.31 |
| MOTA | 948 | С | GLN | 124 | -13.820 | 13.350 | 44.815 | 1.00 18.29 |
| ATOM | 949 | 0 | GLN | 124 | -14.045 | 12.439 | 45.621 | 1.00 17.54 |
| ATOM | 950 | N | MET | 125 | -13.218 | 13.151 | 43.648 | 1.00 16.58 |
| MOTA | 951 | CA | MET | 125 | -12.798 | 11.820 | 43.239 | 1.00 17.11 |
| MOTA | 952 | СВ | MET | 125 | -12.553 | 11.792 | 41.725 | 1.00 17.13 |
| | - | . — | | | | | | |

| MOTA | 953 | CG | MET | 125 | -13.843 | 12.007 | 40.930 | 1.00 20.76 |
|--------------|------------|----------|------------|-----|---------|------------------|----------|------------|
| MOTA | 954 | SD | MET | 125 | -13.598 | 12.024 | 39.156 | 1.00 21.82 |
| ATOM | 955 | CE | MET | 125 | -13.472 | 10.274 | 38.825 | 1.00 24.59 |
| ATOM | 956 | С | MET | 125 | -11.578 | 11.317 | 44.011 | 1.00 15.45 |
| ATOM | 957 | Ō | MET | 125 | -11.513 | 10.143 | 44.357 | 1.00 15.81 |
| ATOM | 958 | N | LEU | 126 | -10.618 | 12.192 | 44.283 | 1.00 15.52 |
| ATOM | 959 | CA | LEU | 126 | -9.458 | 11.776 | 45.047 | 1.00 16.42 |
| MOTA | 960 | CB | LEU | 126 | -8.486 | 12.941 | 45.215 | 1.00 15.46 |
| ATOM | 961 | CG | LEU | 126 | -7.491 | 13.096 | 44.056 | 1.00 16.54 |
| ATOM | 962 | | LEU | 126 | -6.769 | 14.429 | 44.166 | 1.00 17.29 |
| ATOM | 963 | | LEU | 126 | -6.498 | 11.933 | 44.100 | 1.00 17.23 |
| | 964 | CDZ | LEU | 126 | -9.914 | 11.264 | 46.416 | 1.00 10.74 |
| ATOM ATOM | 965 | 0 | LEU | 126 | -9.459 | 10.217 | 46.882 | 1.00 17.03 |
| | | N | | 127 | -10.831 | 12.001 | 47.043 | 1.00 13.07 |
| ATOM | 966 | | THR | 127 | -10.831 | | 47.043 | 1.00 18.88 |
| ATOM | 967 968 | CA CB | THR THR | 127 | -12.489 | 11.648 | 48.788 | 1.00 22.38 |
| ATOM | 969 | | | 127 | | 12.630 13.967 | 48.825 | 1.00 24.31 |
| ATOM | | OG1 | | | -11.971 | | | |
| ATOM | 970 | CG2 | | 127 | -13.018 | 12.265 | 50.167 | 1.00 28.58 |
| ATOM | 971 | C | THR | 127 | -11.950 | 10.235 | 48.406 | 1.00 21.91 |
| ATOM | 972 | 0 | THR | 127 | -11.594 | 9.439 | 49.279 | 1.00 20.97 |
| ATOM | 973 | N | GLU | 128 | -12.854 | | . 47.482 | 1.00 23.67 |
| ATOM | 974 | CA | GLU | 128 | -13.455 | 8.589 | 47.473 | 1.00 22.51 |
| ATOM | 975 | CB | GLU | 128 | -14.643 | 8.532 | 46.499 | 1.00 26.49 |
| ATOM | 976 | CG | GLU | 128 | -14.656 | 9.613 | 45.450 | 1.00 27.76 |
| MOTA | 977 | CD | GLU | 128 | -15.846 | 9.512 | 44.501 | 1.00 26.90 |
| ATOM | 978 | | GLU | 128 | -17.002 | 9.469 | 44.969 | 1.00 26.96 |
| ATOM | 979 | | GLU | 128 | -15.625 | 9.488 | 43.281 | 1.00 26.94 |
| MOTA | 980 | С | GLU | 128 | -12.435 | 7.505 | 47.140 | 1.00 22.91 |
| MOTA | 981 | 0 | GLU | 128 | -12.641 | 6.333 | 47.458 | 1.00 22.08 |
| MOTA | 982 | N | ARG | 129 | -11.324 | 7.895 | 46.520 | 1.00 19.89 |
| ATOM | 983 | CA | ARG | 129 | -10.291 | 6.929 | 46.176 | 1.00 19.15 |
| ATOM | 984 | CB | ARG | 129 | -9.713 | 7.256 | 44.792 | 1.00 18.25 |
| MOTA | 985 | CG | ARG | 129 | -10.712 | 6.934 | 43.664 | 1.00 18.33 |
| MOTA | 986 | CD | ARG | 129 | -10.483 | 7.728 | 42.382 | 1.00 16.74 |
| ATOM | 987 | NE | ARG | 129 | -11.514 | 7.426 | 41.386 | 1.00 14.27 |
| ATOM | 988 | CZ | ARG | 129 | -12.793 | 7.779 | 41.491 | 1.00 16.92 |
| MOTA | 989 | NH1 | ARG | 129 | -13.220 | 8.459 | 42.547 | 1.00 14.64 |
| ATOM | 990 | NH2 | ARG | 129 | -13.654 | 7.440 | 40.544 | 1.00 15.04 |
| MOTA | 991 | С | ARG | 129 | -9.202 | 6.856 | 47.260 | 1.00 19.41 |
| ATOM | 992 | 0 | ARG | 129 | -8.045 | 6.521 | 46.987 | 1.00 18.30 |
| ATOM | 993 | N | ALA | 130 | -9.616 | 7.174 | 48.488 | 1.00 19.07 |
| ATOM | 994 | CA | ALA | 130 | -8.789 | 7.129 | 49.697 | 1.00 17.95 |
| MOTA | 995 | CB | ALA | 130 | -8.201 | 5.722 | 49.868 | 1.00 16.84 |
| ATOM | 996 | С | ALA | 130 | -7.674 | 8.164 | 49.860 | 1.00 18.35 |
| ATOM | 997 | 0 | ALA | 130 | -6.821 | 8.015 | 50.738 | 1.00 17.72 |
| MOTA | 998 | N | VAL | 131 | -7.684 | 9.211 | 49.043 | 1.00 18.16 |
| ATOM | 999 | CA | VAL | 131 | -6.656 | 10.236 | 49.123 | 1.00 18.21 |
| ATOM | 1000 | CB | VAL | 131 | -6.059 | 10.538 | 47.733 | 1.00 18.83 |
| ATOM | 1001 | CG1 | VAL | 131 | -4.972 | 11.599 | 47.856 | 1.00 19.02 |
| ATOM | 1002 | CG2 | VAL | 131 | -5.502 | 9.264 | 47.124 | 1.00 18.78 |
| MOTA | 1003 | C · | VAL | 131 | -7.162 | 11.550 | 49.704 | 1.00 17.21 |
| MOTA | 1004 | 0 | VAL | 131 | -7.921 | 12.274 | 49.059 | 1.00 17.48 |
| ATOM | 1005 | N | PRO | 132 | -6.768 | 11.858 | 50.947 | 1.00 17.96 |
| ATOM | 1006 | CD | PRO | 132 | -6.078 | 10.981 | 51.909 | 1.00 16.97 |
| MOTA | 1007 | CA | PRO | 132 | -7.195 | 13.109 | 51.580 | 1.00 16.82 |
| MOTA | 1008 | CB | PRO | 132 | -6.775 | 12.929 | 53.043 | 1.00 17.66 |
| ATOM | 1009 | CG | PRO | 132 | -5.667 | 11.944 | 52.979 | 1.00 22.79 |
| MOTA | 1010 | С | PRO | 132 | -6.495 | 14.270 | 50.880 | 1.00 16.36 |
| MOTA | 1011 | 0 | PRO | 132 | -5.335 | 14.159 | 50.465 | 1.00 14.89 |
| MOTA | 1012 | N | VAL | 133 | -7.207 | 15.381 | 50.745 | 1.00 15.39 |
| ATOM | 1013 | CA | VAL | 133 | -6.666 | 16.534 | 50.046 | 1.00 14.12 |
| MOTA | 1014 | CB | VAL | 133 | -7.488 | 16.816 | 48.772 | 1.00 14.52 |
| ATOM | 1015 | CG1 | VAL | 133 | -6.921 | 18.016 | 48.037 | 1.00 12.24 |
| MOTA | 1016 | CG2 | | 133 | -7.495 | 15.576 | 47.874 | 1.00 13.02 |
| MOTA | 1017 | С | VAL | 133 | -6.621 | 17.821 | 50.855 | 1.00 14.73 |
| MOTA | 1018 | 0 | VAL | 133 | -7.526 | 18.116 | 51.632 | 1.00 14.95 |
| MOTA | 1019 | N | CYS | 134 | -5.546 | 18.571 | 50.650 | 1.00 15.49 |
| MOTA | 1020 | CA | CYS | 134 | -5.355 | 19.868 | 51.273 | 1.00 14.56 |
| MOTA | 1021 | CB | CYS | 134 | -4.001 | 19.946 | 51.985 | 1.00 14.83 |
| MOTA | 1022 | SG | CYS | 134 | -3.649 | 21.586 | 52.681 | 1.00 17.18 |
| MOTA | 1023 | С | CYS | 134 | -5.388 | 20.866 | 50.121 | 1.00 16.54 |
| MOTA | 1024 | 0 | CYS | 134 | -4.642 | 20.734 | 49.143 | 1.00 16.64 |
| MOTA | 1025 | N | GLY | 135 | -6.276 | 21.851 | 50.215 | 1.00 16.38 |
| MOTA | 1026 | CA | GLY | 135 | -6.371 | 22.864 | 49.176 | 1.00 16.44 |
| MOTA | 1027 | С | GLY | 135 | -5.297 | 23.919 | 49.363 | 1.00 18.40 |
| MOTA | 1028 | 0 | GLY | 135 | -4.615 | | 50.387 | 1.00 17.99 |
| MOTA | 1029 | N | HIS | 136 | -5.150 | 24.806 | 48.382 | 1.00 18.50 |

| MOTA | 1030 | CA | HIS | 136 | -4.147 | 25.868 | 48.435 | 1.00 18.97 |
|------|------|------|-----|-------|--------|------------------|------------------|------------|
| ATOM | 1031 | С | HIS | 136 | -4.624 | 27.055 | 47.603 | 1.00 21.58 |
| ATOM | 1032 | 0 | HIS | 136 | -4.727 | 26.965 | 46.380 | 1.00 21.19 |
| ATOM | 1033 | СВ | HIS | 136 | -2.810 | 25.332 | 47.899 | 1.00 19.18 |
| ATOM | 1034 | CG . | | 136 | -1.638 | 26.240 | 48.126 | 1.00 19.85 |
| ATOM | 1035 | ND1 | | 136 | -0.349 | 25.774 | 48.029 | 1.00 21.61 |
| ATOM | 1036 | CE1 | | 136 | 0.428 | 26.819 | 48.243 | 1.00 22.89 |
| ATOM | 1037 | CD2 | | 136 | -1.614 | 27.568 | 48.403 | 1.00 19.60 |
| | 1037 | NE2 | | 136 | -0.291 | 27.929 | 48.474 | 1.00 20.06 |
| MOTA | | | | | -4.925 | | | 1.00 23.56 |
| MOTA | 1039 | N | LEU | 137 | | 28.162 | 48.278 | |
| MOTA | 1040 | CA | LEU | 137 | -5.399 | 29.374 | 47.617 | 1.00 24.34 |
| MOTA | 1041 | CB | LEU | 137 | -6.850 | 29.655 | 48.019 | 1.00 25.33 |
| MOTA | 1042 | CG | LEU | 137 | -7.884 | 28.574 | 47.685 | 1.00 24.22 |
| MOTA | 1043 | | LEU | 137 | -9.203 | 28.871 | 48.386 | 1.00 24.72 |
| MOTA | 1044 | CD2 | LEU | 137 | -8.072 | 28.510 | 46.181 | 1.00 24.79 |
| ATOM | 1045 | С | LEU | 137 | -4.528 | 30.578 | 47.979 | 1.00 26.25 |
| ATOM | 1046 | 0 | LEU | 137 | -3.798 | 30.552 | 48.969 | 1.00 25.52 |
| MOTA | 1047 | N | GLY | 138 | -4.617 | 31.630 | 47.169 | 1.00 28.18 |
| ATOM | 1048 | CA | GLY | 138 | -3.837 | 32.827 | 47.411 | 1.00 30.33 |
| ATOM | 1049 | C | GLY | 138 | -2.702 | 32.926 | 46.414 | 1.00 32.93 |
| ATOM | 1050 | 0 | GLY | 138 | -2.919 | 32.829 | 45.208 | 1.00 33.34 |
| ATOM | 1051 | N | LEU | 139 | -1.489 | 33.109 | 46.916 | 1.00 34.19 |
| ATOM | 1052 | CA | LEU | 139 | -0.320 | 33.212 | 46.058 | 1.00 36.17 |
| ATOM | 1053 | CB | LEU | 139 | 0.784 | 33.982 | 46.787 | 1.00 37.11 |
| ATOM | 1054 | CG | LEU | 139 | 1.968 | 34.522 | 45.977 | 1.00 39.03 |
| ATOM | 1055 | | LEU | 139 | 2.838 | 35.383 | 46.884 | 1.00 40.33 |
| ATOM | 1056 | | LEU | 139 | 2.780 | 33.385 | 45.383 | 1.00 37.65 |
| ATOM | 1057 | C | LEU | 139 | 0.157 | 31.803 | 45.698 | 1.00 37.33 |
| ATOM | 1058 | 0 | LEU | 139 | 0.914 | 31.184 | 46.442 | 1.00 37.46 |
| ATOM | 1059 | N | THR | 140 | -0.304 | 31.303 | 44.555 | 1.00 37.52 |
| | | | THR | 140 | 0.064 | 29.974 | 44.081 | 1.00 37.52 |
| MOTA | 1060 | CA | | 140 | | 29.367 | | 1.00 38.36 |
| ATOM | 1061 | CB | THR | | -1.057 | | 43.214 | |
| MOTA | 1062 | | THR | 140 | -1.375 | 30.266 | 42.145 | 1.00 38.58 |
| ATOM | 1063 | CG2 | THR | 140 | -2.302 | 29.118 | 44.053 | 1.00 38.94 |
| MOTA | 1064 | С | THR | 140 | 1.343 | 30.044 | 43.249 | 1.00 38.97 |
| MOTA | 1065 | 0 | THR | 140 | 1.314 | 30.444 | 42.085 | 1.00 39.39 |
| ATOM | 1066 | N | PRO | 141 | 2.483 | 29.646 | 43.837 | 1.00 38.90 |
| MOTA | 1067 | CD | PRO | 141 | 2.619 | 29.077 | 45.190 | 1.00 39.41 |
| MOTA | 1068 | CA | PRO | 141 | 3.778 | 29.669 | 43.147 | 1.00 37.89 |
| MOTA | 1069 | CB | PRO | 141 | 4.742 | 29.115 | 44.197 | 1.00 38.82 |
| MOTA | 1070 | CG | PRO | 141 | 3.864 | 28.250 | 45.055 | 1.00 40.43 |
| MOTA | 1071 | C | PRO | 141 | 3.831 | 28.899 | 41.831 | 1.00 37.49 |
| ATOM | 1072 | 0 | PRO | 141 | 4.622 | 29.233 | 40.947 | 1.00 34.97 |
| ATOM | 1073 | N | GLN | 142 | 2.997 | 27.872 | 41.700 | 1.00 35.93 |
| MOTA | 1074 | CA | GLN | 142 | 2.975 | 27.084 | 40.470 | 1.00 37.63 |
| ATOM | 1075 | CB | GLN | 142 | 2.072 | 25.855 | 40.635 | 1.00 35.67 |
| ATOM | 1076 | CG | GLN | 142 | 2.807 | 24.600 | 41.091 | 1.00.34.13 |
| ATOM | 1077 | CD | GLN | 142 | 1.860 | 23.471 | 41.458 | 1.00 33.64 |
| ATOM | 1078 | OE1 | | 142 | 0.906 | 23.186 | 40.737 | 1.00 31.98 |
| ATOM | 1079 | NE2 | | 142 | 2.127 | 22.817 | 42.583 | 1.00 33.66 |
| ATOM | 1080 | С | GLN | 142 | 2.508 | 27.920 | 39.282 | 1.00 38.52 |
| ATOM | 1081 | ō | GLN | 142 | 2.859 | 27.635 | 38.134 | 1.00 38.49 |
| ATOM | 1082 | N | SER | 143 | 1.718 | 28.953 | 39.562 | 1.00 39.73 |
| ATOM | 1083 | CA | SER | 143 | 1.210 | 29.834 | 38.513 | 1.00 40.92 |
| ATOM | 1084 | СВ | SER | 143 | -0.279 | 30.123 | 38.732 | 1.00 40.43 |
| ATOM | 1085 | OG | SER | 143 | -1.059 | 28.946 | 38.606 | 1.00 41.04 |
| ATOM | 1086 | C | SER | 143 | 1.982 | 31.149 | 38.484 | 1.00 41.64 |
| ATOM | 1087 | ō | SER | 143 | 1.448 | 32.178 | 38.076 | 1.00 42.46 |
| ATOM | 1088 | N | VAL | 144 | 3.238 | 31.110 | 38.916 | 1.00 42.62 |
| ATOM | 1089 | CA | VAL | 144 | 4.075 | 32.306 | 38.935 | 1.00 43.78 |
| ATOM | 1099 | CB | VAL | 144 | 5.483 | 31.995 | 39.492 | 1.00 43.70 |
| ATOM | 1090 | CG1 | | 144 | 6.194 | 31.001 | 38.588 | 1.00 43.74 |
| | | | | | 6.291 | | 39.616 | 1.00 44.06 |
| ATOM | 1092 | CG2 | | 144 | 4.219 | 33.278 32.918 | 37.541 | 1.00 44.08 |
| MOTA | 1093 | C | VAL | 144 | | | | |
| ATOM | 1094 | 0 | VAL | 144 . | 4.423 | 34.123 | 37.405 36.512 | 1.00 44.39 |
| MOTA | 1095 | N | ASN | 145 | 4.111 | 32.082 | | 1.00 45.34 |
| ATOM | 1096 | CA | ASN | 145 | 4.231 | 32.540 | 35.130 | 1.00 47.01 |
| ATOM | 1097 | CB | ASN | 145 | 4.606 | 31.368 | 34.214 | 1.00 47.34 |
| ATOM | 1098 | CG | ASN | 145 | 5.992 | 30.821 | 34.505 | 1.00 48.01 |
| ATOM | 1099 | OD1 | | 145 | 7.000 | 31.488 | 34.264 | 1.00 47.54 |
| MOTA | 1100 | | ASN | 145 | 6.049 | 29.602 | 35.031 | 1.00 48.81 |
| MOTA | 1101 | С | ASN | 145 | 2.938 | 33.179 | 34.640 | 1.00 47.35 |
| MOTA | 1102 | 0 | ASN | 145 | 2.905 | 33.813 | 33.585 | 1.00 47.69 |
| MOTA | 1103 | N | ILE | 146 | 1.872 | 33.005 | 35.410 | 1.00 48.31 |
| MOTA | 1104 | CA | ILE | 146 | 0.578 | 33.569 | 35.055 | 1.00 49.69 |
| MOTA | 1105 | CB | ILE | 146 | -0.574 | 32.693 | 35.589 | 1.00 49.13 |
| MOTA | 1106 | CG2 | ILE | 146 | -1.912 | 33.335 | 35.263 | 1.00 48.60 |
| | | | | | | | | |

| ATOM | 1107 | CG1 | ILE | 146 | -0.485 | 31.290 | 34.981 | 1.00 48.60 |
|------|------|-----|-----|------------------|---------|--------|--------|------------|
| ATOM | 1108 | CD1 | ILE | 146 | -0.628 | 31.262 | 33.472 | 1.00 48.16 |
| ATOM | 1109 | С | ILE | 146 | 0.426 | 34.976 | 35.623 | 1.00 51.32 |
| АТОМ | 1110 | 0 | ILE | 146 | -0.045 | 35.880 | 34.934 | 1.00 51.26 |
| ATOM | 1111 | N | PHE | 147 | 0.831 | 35.154 | 36.879 | 1.00 52.78 |
| ATOM | 1112 | CA | PHE | 147 | 0.738 | 36.448 | 37.553 | 1.00 54.17 |
| | | | | | | | | |
| ATOM | 1113 | CB | PHE | 147 | 0.713 | 36.254 | 39.072 | 1.00 55.12 |
| MOTA | 1114 | CG | PHE | 147 | -0.198 | 35.152 | 39.528 | 1.00 56.36 |
| MOTA | 1115 | | PHE | 147 | -1.553 | 35.177 | 39.218 | 1.00 57.26 |
| MOTA | 1116 | CD2 | | 147 | 0.303 | 34.084 | 40.266 | 1.00 57.27 |
| MOTA | 1117 | CE1 | PHE | 147 | -2.400 | 34.151 | 39.634 | 1.00 57.90 |
| MOTA | 1118 | CE2 | PHE | 147 | -0.533 | 33.052 | 40.688 | 1.00 57.81 |
| MOTA | 1119 | CZ | PHE | 147 | -1.887 | 33.086 | 40.371 | 1.00 58.12 |
| ATOM | 1120 | С | PHE | 147 | 1.914 | 37.350 | 37.188 | 1.00 54.46 |
| ATOM | 1121 | 0 | PHE | 147 | 1.937 | 38.528 | 37.544 | 1.00 54.14 |
| ATOM | 1122 | N | GLY | 148 | 2.890 | 36.787 | 36.483 | 1.00 55.28 |
| ATOM | 1123 | CA | GLY | 148 | 4.056 | 37.555 | 36.090 | 1.00 56.16 |
| ATOM | 1124 | C | GLY | 148 | 4.972 | 37.817 | 37.268 | 1.00 56.63 |
| ATOM | 1125 | ō | GLY | 148 | 5.699 | 38.809 | 37.294 | 1.00 56.49 |
| | 1126 | | GLY | 149 | 4.933 | 36.920 | 38.249 | 1.00 57.50 |
| ATOM | | N | | | | | | |
| MOTA | 1127 | CA | GLY | 149 | 5.761 | 37.068 | 39.431 | 1.00 58.67 |
| MOTA | 1128 | C | GLY | 149 | 4.997 | 36.690 | 40.685 | 1.00 59.94 |
| ATOM | 1129 | 0 | GLY | 149 | 3.828 | 36.305 | 40.613 | 1.00 59.46 |
| MOTA | 1130 | N | TYR | 150 | 5.653 | 36.797 | 41.837 | 1.00 61.00 |
| ATOM | 1131 | CA | TYR | 150 | 5.018 | 36.467 | 43.108 | 1.00 62.09 |
| MOTA | 1132 | CB | TYR | 150 | 6.029 | 35.830 | 44.068 | 1.00 62.64 |
| ATOM | 1133 | CG | TYR | 150 | 6.779 | 34.653 | 43.484 | 1.00 63.79 |
| ATOM | 1134 | CD1 | TYR | 150 | 7-910 | 34.846 | 42.688 | 1.00 64.15 |
| MOTA | 1135 | CE1 | TYR | 150 | 8.601 | 33.764 | 42.142 | 1.00 64.08 |
| MOTA | 1136 | CD2 | TYR | 150 | 6.355 | 33.344 | 43.718 | 1.00 64.03 |
| ATOM | 1137 | CE2 | TYR | 150 | 7.038 | 32.256 | 43.175 | 1.00 63.87 |
| ATOM | 1138 | CZ | TYR | 150 | 8.160 | 32.474 | 42.389 | 1.00 64.27 |
| ATOM | 1139 | ОН | TYR | 150 ~ | 8.840 | 31.407 | 41.849 | 1.00 64.43 |
| ATOM | 1140 | C | TYR | 150 | 4.426 | 37.721 | 43.744 | 1.00 62.40 |
| ATOM | 1141 | 0 | TYR | 150 | 5.141 | 38.523 | 44.347 | 1.00 62.40 |
| | | | | | | | | |
| ATOM | 1142 | N | LYS | 151 | 3.113 | 37.883 | 43.603 | 1.00 62.64 |
| MOTA | 1143 | CA | LYS | 151 | 2.414 | 39.038 | 44.152 | 1.00 62.63 |
| MOTA | 1144 | CB | LYS | 151 | 1.768 | 39.842 | 43.020 | 1.00 63.52 |
| MOTA | 1145 | CG | LYS | 151 | 2.765 | 40.359 | 41.993 | 1.00 64.61 |
| MOTA | 1146 | CD | LYS | 151 | 2.085 | 41.186 | 40.916 | 1.00 65.48 |
| MOTA | 1147 | CE | LYS | 151 | 3.100 | 41.731 | 39.921 | 1.00 66.46 |
| MOTA | 1148 | NZ | LYS | 151 | 2.464 | 42.586 | 38.878 | 1.00 66.97 |
| MOTA | 1149 | C | LYS | 151 | 1.351 | 38.615 | 45.161 | 1.00 62.18 |
| MOTA | 1150 | 0 | LYS | 151 | 1.022 | 37.433 | 45.273 | 1.00 62.06 |
| ATOM | 1151 | N | VAL | 152 | 0.815 | 39.586 | 45.893 | 1.00 61.53 |
| ATOM | 1152 | CA | VAL | 152 | -0.204 | 39.309 | 46.897 | 1.00 60.97 |
| ATOM | 1153 | CB | VAL | 152 | -0.190 | 40.378 | 48.010 | 1.00 60.76 |
| ATOM | 1154 | CG1 | | 152 | -1.225 | 40.039 | 49.073 | 1.00 60.74 |
| ATOM | 1155 | CG2 | | 152 | 1.195 | 40.468 | 48.624 | 1.00 60.69 |
| ATOM | | | | | | | | |
| | 1156 | C | VAL | 152 | -1.601 | 39.263 | 46.293 | 1.00 60.64 |
| MOTA | 1157 | 0 | VAL | 152 ⁻ | -1.999 | 40.166 | 45.559 | 1.00 60.43 |
| ATOM | 1158 | N | GLN | 153 | -2.341 | 38.205 | 46.608 | 1.00 60.42 |
| ATOM | 1159 | CA | GLN | 153 | -3.703 | 38.042 | 46.111 | 1.00 60.14 |
| ATOM | 1160 | CB | GLN | 153 | -3.918 | 36.620 | 45.581 | 1.00 60.93 |
| ATOM | 1161 | CG | GLN | 153 | -3.467 | 36.402 | 44.140 | 1.00 61.33 |
| MOTA | 1162 | CD | GLN | 153 | -1.977 | 36.593 | 43.953 | 1.00 61.41 |
| MOTA | 1163 | OE1 | GLN | 153 | -1.169 | 35.901 | 44.572 | 1.00 62.43 |
| MOTA | 1164 | NE2 | GLN | 153 . | ~1.605 | 37.531 | 43.091 | 1.00 60.96 |
| MOTA | 1165 | С | GLN | 153 | -4.715 | 38.333 | 47.214 | 1.00 59.42 |
| ATOM | 1166 | 0 | GLN | 153 | -4.350 | 38.483 | 48.379 | 1.00 59.06 |
| ATOM | 1167 | N | GLY | 154 | -5.988 | 38.410 | 46.838 | 1.00 58.76 |
| ATOM | 1168 | CA | GLY | 154 | -7.030 | 38.685 | 47.808 | 1.00 58.28 |
| ATOM | 1169 | C | GLY | 154 | -7.425 | 40.149 | 47.825 | 1.00 57.80 |
| ATOM | 1170 | o | GLY | 154 | -8.548 | 40.489 | 48.199 | 1.00 56.85 |
| ATOM | 1171 | N | ARG | 155 | -6.497 | 41.013 | 47.421 | 1.00 58.06 |
| | 1172 | | | | -6.732 | | | 1.00 58.09 |
| ATOM | | CA | ARG | 155 | | 42.455 | 47.380 | |
| ATOM | 1173 | CB | ARG | 155 | -5.535 | 43.174 | 46.742 | 1.00 59.37 |
| ATOM | 1174 | CG | ARG | 155 | -4.204 | 42.996 | 47.470 | 1.00 60.93 |
| ATOM | 1175 | CD | ARG | 155 | -4.242 | 43.586 | 48.873 | 1.00 62.00 |
| ATOM | 1176 | NE | ARG | 155 | -2.977 | 43.409 | 49.587 | 1.00 62.99 |
| ATOM | 1177 | cz | ARG | 155 | -1.826 | 43.969 | 49.227 | 1.00 63.25 |
| MOTA | 1178 | | ARG | 155 | -1.773 | 44.750 | 48.157 | 1.00 63.93 |
| ATOM | 1179 | NH2 | ARG | 155 | -0.727 | 43.753 | 49.938 | 1.00 63.47 |
| ATOM | 1180 | С | ARG | 155 | -7.990 | 42.771 | 46.575 | 1.00 57.05 |
| MOTA | 1181 | 0 | ARG | 155 | -8.123 | 42.355 | 45.425 | 1.00 57.28 |
| ATOM | 1182 | N | GLY | 156 | -8.908 | 43.513 | 47.184 | 1.00 55.32 |
| ATOM | 1183 | CA | GLY | 156 | -10.136 | 43.862 | 46.498 | 1.00 53.27 |
| | | | | | | | | |

| ATOM | 1184 | С | GLY | 156 | -11.306 | 43.028 | 46.976 | 1.00 52.09 |
|------|------|-----|----------------------|-----|---------|--------|--------|------------|
| ATOM | 1185 | 0 | GLY | 156 | -11.123 | 41.930 | 47.501 | 1.00 51.92 |
| ATOM | 1186 | N | ASP | 157 | -12.511 | 43.553 | 46.790 | 1.00 50.40 |
| MOTA | 1187 | CA | ASP | 157 | -13.731 | 42.872 | 47.208 | 1.00 49.29 |
| | 1188 | CB | | 157 | -14.914 | | 47.090 | 1.00 49.29 |
| MOTA | | | ASP | | | 43.832 | | |
| MOTA | 1189 | CG | ASP | 157 | -14.693 | 45.121 | 47.854 | 1.00 51.46 |
| MOTA | 1190 | OD1 | | 157 | -14.893 | 45.122 | 49.086 | 1.00 50.41 |
| MOTA | 1191 | OD2 | ASP | 157 | -14.304 | 46.126 | 47.216 | 1.00 53.02 |
| ATOM | 1192 | С | ASP | 157 | -13.991 | 41.634 | 46.358 | 1.00 48.08 |
| MOTA | 1193 | 0 | ASP | 157 | -14.231 | 40.544 | 46.881 | 1.00 46.48 |
| ATOM | 1194 | N | GLU | 158 | -13.942 | 41.813 | 45.043 | 1.00 46.08 |
| ATOM | 1195 | CA | GLU | 158 | -14.178 | 40.718 | 44.116 | 1.00 45.63 |
| | | | | | | | | |
| MOTA | 1196 | CB | GLU | 158 | -14.092 | 41.225 | 42.675 | 1.00 48.09 |
| MOTA | 1197 | CG | GLU | 158 | -14.387 | 40.169 | 41.626 | 1.00 50.76 |
| MOTA | 1198 | CD | GLU | 158 | -14.503 | 40.755 | 40.233 | 1.00 53.13 |
| ATOM | 1199 | OE1 | GLU | 158 | -15.430 | 41.564 | 40.002 | 1.00 55.10 |
| ATOM | 1200 | OE2 | GLU | 158 | -13.670 | 40.411 | 39.367 | 1.00 54.38 |
| ATOM | 1201 | С | GLU | 158 | -13.187 | 39.578 | 44.329 | 1.00 43.56 |
| ATOM | 1202 | 0 | GLU | 158 | -13.584 | 38.429 | 44.529 | 1.00 42.93 |
| ATOM | 1203 | N | ALA | 159 | -11.898 | 39.899 | 44.287 | 1.00 41.57 |
| | 1204 | CA | ALA | 159 | -10.859 | 38.893 | 44.482 | 1.00 39.78 |
| ATOM | | | | | | | | |
| ATOM | 1205 | CB | ALA | 159 | -9.482 | 39.547 | 44.444 | 1.00 39.93 |
| ATOM | 1206 | С | ALA | 159 | -11.065 | 38.177 | 45.814 | 1.00 38.91 |
| MOTA | 1207 | О | ALA | 159 | -10.917 | 36.958 | 45.904 | 1.00 37.78 |
| ATOM | 1208 | N | GLY | 160 | -11.419 | 38.944 | 46.840 | 1.00 36.56 |
| ATOM | 1209 | CA | GLY | 160 | -11.642 | 38.371 | 48.152 | 1.00 35.21 |
| ATOM | 1210 | С | GLY | 160 | -12.818 | 37.416 | 48.194 | 1.00 35.10 |
| ATOM | 1211 | O | GLY | 160 | -12.718 | 36.330 | 48.768 | 1.00 34.10 |
| ATOM | 1212 | N | ASP | 161 | -13.935 | 37.813 | 47.591 | 1.00 33.83 |
| | | | | 161 | | 36.971 | 47.575 | 1.00 33.55 |
| ATOM | 1213 | CA | ASP | | -15.126 | | | |
| MOTA | 1214 | CB | ASP | 161 | -16.335 | 37.747 | 47.038 | 1.00 34.86 |
| ATOM | 1215 | CG | ASP | 161 | -16.651 | 38.986 | 47.861 | 1.00 35.97 |
| MOTA | 1216 | OD1 | ASP | 161 | -16.702 | 38.890 | 49.109 | 1.00 34.80 |
| ATOM | 1217 | OD2 | ASP | 161 | -16.862 | 40.056 | 47.255 | 1.00 37.49 |
| ATOM | 1218 | С | ASP | 161 | -14.897 | 35.727 | 46.718 | 1.00 32.66 |
| MOTA | 1219 | 0 | ASP | 161 | -15.553 | 34.704 | 46.910 | 1.00 30.79 |
| ATOM | 1220 | N | GLN | 162 | -13.967 | 35.822 | 45.773 | 1.00 33.43 |
| ATOM | 1221 | CA | GLN | 162 | -13.657 | 34.696 | 44.901 | 1.00 34.32 |
| | | | | | | | 43.712 | 1.00 35.93 |
| MOTA | 1222 | CB | GLN | 162 | -12.810 | 35.160 | | |
| MOTA | 1223 | CG | GLN | 162 | -12.549 | 34.069 | 42.680 | 1.00 40.84 |
| MOTA | 1224 | CD | GLN | 162 | -13.827 | 33.377 | 42.235 | 1.00 43.13 |
| ATOM | 1225 | OE1 | GLN | 162 | -14.770 | 34.023 | 41.774 | 1.00 45.74 |
| ATOM | 1226 | NE2 | GLN | 162 | -13.866 | 32.056 | 42.374 | 1.00 44.65 |
| MOTA | 1227 | С | GLN | 162 | ~12.915 | 33.613 | 45.683 | 1.00 32.85 |
| MOTA | 1228 | 0 | GLN | 162 | -13.236 | 32.429 | 45.575 | 1.00 32.77 |
| ATOM | 1229 | N | LEU | 163 | -11.928 | 34.022 | 46.474 | 1.00 31.71 |
| ATOM | 1230 | CA | LEU | 163 | -11.159 | 33.074 | 47.275 | 1.00 31.82 |
| ATOM | 1231 | CB | LEU | 163 | -10.025 | 33.792 | 48.017 | 1.00 33.87 |
| | | | | | | | | |
| ATOM | 1232 | CG | LEU | 163 | -8.879 | 34.358 | 47.173 | 1.00 35.14 |
| MOTA | 1233 | | LEU | 163 | -7.918 | 35.131 | 48.064 | 1.00 36.34 |
| ATOM | 1234 | CD2 | LEU | 163 | -8.146 | 33.222 | 46.472 | 1.00 36.72 |
| MOTA | 1235 | C | LEU | 163 | -12.059 | 32.363 | 48.279 | 1.00 31.54 |
| ATOM | 1236 | 0 | LEU | 163 | -11.968 | 31.150 | 48.456 | 1.00 30.72 |
| MOTA | 1237 | N | LEU | 164 | -12.932 | 33.124 | 48.934 | 1.00 30.37 |
| ATOM | 1238 | CA | LEU | 164 | -13.848 | 32.556 | 49.915 | 1.00 29.45 |
| ATOM | 1239 | СВ | LEU | 164 | -14.702 | 33.669 | 50.530 | 1.00 31.08 |
| ATOM | 1240 | CG | LEU | 164 | -15.296 | 33.451 | 51.925 | 1.00 31.21 |
| | | | LEU | 164 | -16.045 | 34.715 | 52.346 | 1.00 35.31 |
| ATOM | 1241 | | | | -16.218 | | | |
| ATOM | 1242 | | LEU | 164 | | 32.261 | 51.937 | 1.00 32.29 |
| ATOM | 1243 | C | LEU | 164 | -14.737 | 31.540 | 49.203 | 1.00 28.86 |
| ATOM | 1244 | 0 | LEU | 164 | -15.058 | 30.480 | 49.744 | 1.00 28.39 |
| MOTA | 1245 | N | SER | 165 | -15.126 | 31.876 | 47.978 | 1.00 27.45 |
| MOTA | 1246 | CA | SER | 165 | -15.973 | 31.004 | 47.173 | 1.00 28.46 |
| ATOM | 1247 | CB | SER | 165 | -16.356 | 31.709 | 45.867 | 1.00 26.87 |
| ATOM | 1248 | OG | SER | 165 | -17.280 | 30.932 | 45.133 | 1.00 31.92 |
| ATOM | 1249 | C | SER | 165 | -15.243 | 29.699 | 46.856 | 1.00 26.43 |
| ATOM | 1250 | ō | SER | 165 | -15.796 | 28.611 | 47.010 | 1.00 27.06 |
| ATOM | 1251 | | | 166 | -13.790 | 29.820 | 46.412 | 1.00 27.00 |
| | | N | ASP | | | | | |
| MOTA | 1252 | CA | ASP | 166 | -13.194 | 28.648 | 46.078 | 1.00 25.84 |
| MOTA | 1253 | CB | ASP | 166 | -11.881 | 29.057 | 45.407 | 1.00 27.39 |
| MOTA | 1254 | CG | ASP | 166 | -12.086 | 29.645 | 44.028 | 1.00 28.71 |
| MOTA | 1255 | | ASP | 166 | -12.913 | 29.099 | 43.262 | 1.00 31.41 |
| MOTA | 1256 | OD2 | ASP | 166 | -11.407 | 30.644 | 43.696 | 1.00 28.72 |
| ATOM | 1257 | С | ASP | 166 | -12.886 | 27.840 | 47.331 | 1.00 25.65 |
| ATOM | 1258 | ō | ASP | 166 | -12.769 | 26.615 | 47.275 | 1.00 25.23 |
| ATOM | 1259 | N | ALA | 167 | -12.750 | 28.534 | 48.459 | 1.00 23.48 |
| ATOM | 1260 | CA | ALA | 167 | -12.454 | 27.893 | 49.733 | 1.00 23.48 |
| AION | 1200 | CH | ΑЦΑ | 107 | -14.434 | 21.033 | 49.133 | 1.00 44.76 |
| | | | | | | | | |

| ATOM | 1261 | CB | ALA | 167 | -12.184 | 28.956 | 50.806 | 1.00 23.00 |
|--------|------|------|-------|-----|---------|--------|--------|------------|
| ATOM | 1262 | С | ALA | 167 | -13.599 | 26.991 | 50.169 | 1.00 21.48 |
| ATOM | 1263 | ō | ALA | 167 | -13.387 | 25.833 | 50.532 | 1.00 19.60 |
| | | | | | | 27.523 | | 1.00 21.01 |
| ATOM | 1264 | N | LEU | 168 | -14.817 | | 50.150 | |
| ATOM | 1265 | CA | LEU | 168 | -15.983 | 26.734 | 50.534 | 1.00 20.93 |
| MOTA | 1266 | CB | LEU | 168 | -17.228 | 27.622 | 50.596 | 1.00 21.15 |
| MOTA | 1267 | CG | LEU | 168 | -17.387 | 28.514 | 51.831 | 1.00 19.76 |
| ATOM | 1268 | CD1 | LEU | 168 | -18.297 | 29.693 | 51.501 | 1.00 21.84 |
| ATOM | 1269 | CD2 | LEU | 168 | -17.967 | 27.699 | 52.978 | 1.00 20.27 |
| ATOM | 1270 | C | LEU | 168 | -16.199 | 25.630 | 49.509 | 1.00 20.35 |
| ATOM | 1271 | õ | LEU | 168 | -16.610 | 24.527 | 49.855 | 1.00 21.26 |
| | | | | 169 | -15.925 | 25.943 | 48.248 | 1.00 21.20 |
| MOTA | 1272 | N | ALA | | | | | |
| MOTA | 1273 | CA | ALA | 169 | -16.088 | 24.984 | 47.161 | 1.00 22.58 |
| ATOM | 1274 | CB | ALA | 169 | -15.774 | 25.648 | 45.829 | 1.00 19.71 |
| MOTA | 1275 | С | ALA | 169 | -15.198 | 23.764 | 47.368 | 1.00 23.26 |
| MOTA | 1276 | 0 | ALA | 169 | -15.638 | 22.626 | 47.192 | 1.00 23.84 |
| ATOM | 1277 | N | LEU | 170 | -13.944 | 24.004 | 47.737 | 1.00 22.11 |
| ATOM | 1278 | CA | LEU | 170 | -13.005 | 22.915 | 47.974 | 1.00 21.77 |
| ATOM | 1279 | СВ | LEU | 170 | -11.585 | 23.473 | 48.169 | 1.00 19.66 |
| ATOM | 1280 | CG | LEU | 170 | -10.934 | 24.127 | 46.939 | 1.00 17.91 |
| | | CD1 | | 170 | -9.666 | 24.896 | 47.340 | 1.00 19.18 |
| MOTA | 1281 | | | | | | | |
| ATOM | 1282 | CD2 | LEU | 170 | ~10.595 | 23.043 | 45.910 | 1.00 18.15 |
| MOTA | 1283 | С | LEU | 170 | -13.447 | 22.114 | 49.198 | 1.00 20.95 |
| MOTA | 1284 | 0 | LEU | 170 | -13.408 | 20.888 | 49.185 | 1.00 20.34 |
| ATOM | 1285 | N | GLU | 171 | -13.883 | 22.803 | 50.253 | 1.00 21.68 |
| MOTA | 1286 | CA | GLU | 171 | -14.332 | 22.116 | 51.461 | 1.00 21.25 |
| MOTA | 1287 | CB | GLU | 171 | -14.746 | 23.129 | 52.536 | 1.00 22.53 |
| ATOM | 1288 | CG | GLU | 171 | -15.385 | 22.502 | 53.775 | 1.00 25.91 |
| ATOM | 1289 | CD | GLU | 171 | -15.745 | 23.536 | 54.834 | 1.00 27.19 |
| ATOM | 1290 | | GLU | 171 | -16.404 | 24.538 | 54.477 | 1.00 27.15 |
| | | | | | | | | |
| ATOM - | 1291 | | GLU | 171 | -15.377 | 23.342 | 56.016 | |
| ATOM | 1292 | C | GLU | 171 | -15.504 | 21.195 | 51.149 | 1.00 21.24 |
| ATOM | 1293 | 0 | GLU . | 171 | -15.538 | 20.044 | 51.592 | 1.00 21.38 |
| ATOM | 1294 | N | ALA | 172 | -16.460 | 21.701 | 50.374 | 1.00 21.12 |
| MOTA | 1295 | CA | ALA | 172 | -17.637 | 20.919 | 50.013 | 1.00 21.23 |
| MOTA | 1296 | CB | ALA | 172 | -18.651 | 21.807 | 49.299 | 1.00 21.68 |
| ATOM | 1297 | С | ALA | 172 | -17.272 | 19.724 | 49.134 | 1.00 20.21 |
| ATOM | 1298 | 0 | ALA | 172 | -17.953 | 18.695 | 49.147 | 1.00 19.47 |
| ATOM | 1299 | N | ALA | 173 | -16.192 | 19.866 | 48.374 | 1.00 22.48 |
| ATOM | 1300 | CA | ALA | 173 | -15.725 | 18.801 | 47.491 | 1.00 19.03 |
| ATOM | 1301 | CB | ALA | 173 | -14.767 | 19.379 | 46.444 | 1.00 20.74 |
| | | | | | | | | |
| MOTA | 1302 | C | ALA | 173 | -15.034 | 17.690 | 48.286 | 1.00 21.09 |
| MOTA | 1303 | 0 | ALA | 173 | -14.845 | 16.575 | 47.792 | 1.00 20.88 |
| ATOM | 1304 | N | GLY | 174 | -14.651 | 18.000 | 49.520 | 1.00 20.56 |
| ATOM | 1305 | CA | GLY | 174 | -14.011 | 16.998 | 50.352 | 1.00 20.44 |
| MOTA | 1306 | С | GLY | 174 | -12.664 | 17.365 | 50.949 | 1.00 19.70 |
| MOTA | 1307 | 0 | GLY | 174 | -12.077 | 16.559 | 51.669 | 1.00 19.40 |
| MOTA | 1308 | N | ALA | 175 | -12.157 | 18.559 | 50.658 | 1.00 20.44 |
| ATOM | 1309 | CA | ALA | 175 | -10.871 | 18.964 | 51.218 | 1.00 19.55 |
| ATOM | 1310 | CB | ALA | 175 | -10.464 | 20.316 | 50.677 | 1.00 20.28 |
| ATOM | 1311 | C | ALA | 175 | -10.972 | 19.006 | 52.747 | 1.00 21.76 |
| | | 0 | | 175 | | | 53.297 | 1.00 20.48 |
| MOTA | 1312 | | ALA | | -11.891 | 19.610 | | |
| ATOM | 1313 | N | GLN | 176 | -10.037 | 18.347 | 53.431 | 1.00 20.03 |
| MOTA | 1314 | CA | GLN | 176 | -10.041 | 18.310 | 54.892 | 1.00 20.58 |
| ATOM | 1315 | CB | GLN | 176 | -9.654 | 16.916 | 55.392 | 1.00 20.99 |
| ATOM | 1316 | CG | GLN | 176 | -10.582 | 15.828 | 54.889 | 1.00 23.71 |
| MOTA | 1317 | CD | GLN | 176 | -10.327 | 14.487 | 55.535 | 1.00 25.55 |
| MOTA | 1318 | OE1 | GLN | 176 | -10.614 | 14.291 | 56.713 | 1.00 29.79 |
| MOTA | 1319 | NE2 | GLN | 176 | -9.785 | 13.554 | 54.766 | 1.00 27.44 |
| ATOM | 1320 | С | GLN | 176 | -9.096 | 19.349 | 55.487 | 1.00 20.58 |
| ATOM | 1321 | 0 | GLN | 176 | -9.021 | 19.515 | 56.705 | 1.00 19.49 |
| ATOM | 1322 | N | LEU | 177 | -8.376 | 20.037 | 54.610 | 1.00 20.99 |
| ATOM | 1323 | CA | LEU | 177 | -7.440 | 21.074 | 55.001 | 1.00 20.99 |
| | | | | | | | | |
| ATOM | 1324 | CB | LEU | 177 | -6.063 | 20.478 | 55.315 | 1.00 22.64 |
| MOTA | 1325 | CG | LEU | 177 | -5.821 | 20.041 | 56.763 | 1.00 25.50 |
| MOTA | 1326 | | | 177 | -4.483 | 19.321 | 56.874 | 1.00 24.79 |
| MOTA | 1327 | | LEU | 177 | -5.838 | 21.272 | 57.670 | 1.00 24.33 |
| MOTA | 1328 | С | LEU | 177 | -7.308 | 22.097 | 53.885 | 1.00 22.00 |
| ATOM | 1329 | 0 | LEU | 177 | -7.529 | 21.792 | 52.709 | 1.00 20.39 |
| MOTA | 1330 | N | LEU | 178 | -6.948 | 23.317 | 54.261 | 1.00 19.35 |
| MOTA | 1331 | CA | LEU | 178 | -6.779 | 24.386 | 53.295 | 1.00 20.42 |
| ATOM | 1332 | CB | LEU | 178 | -8.063 | 25.211 | 53.180 | 1.00 19.08 |
| ATOM | 1333 | CG · | LEU | 178 | -7.947 | 26.457 | 52.297 | 1.00 21.83 |
| ATOM | 1334 | CD1 | | 178 | -7.793 | 26.056 | 50.832 | 1.00 22.51 |
| | | | | | | 27.327 | 52.472 | 1.00 22.31 |
| MOTA | 1335 | CD2 | | 178 | -9.187 | | | |
| ATOM | 1336 | С | LEU | 178 | -5.630 | 25.304 | 53.681 | 1.00 21.17 |
| MOTA | 1337 | 0 | LEU | 178 | -5.499 | 25.703 | 54.838 | 1.00 21.61 |

| ATOM | 1338 | N | VAL | 179 | -4.803 | 25.630 | 52.696 | 1.00 20.87 |
|--------------|--------------|-----------|------------|------------|------------------|------------------|------------------|--------------------------|
| ATOM | 1339 | CA | VAL | 179 | -3.672 | 26.518 | 52.893 | 1.00 21.64 |
| ATOM | 1340 | CB | VAL | 179 | -2.360 | 25.910 | 52.320 | 1.00 21.83 |
| ATOM | 1341 | CG1 | VAL | 179 | -1.280 | 26.985 | 52.238 | 1.00 21.50 |
| ATOM | 1342 | CG2 | VAL | 179 | -1.876 | 24.760 | 53.204 | 1.00 16.70 |
| ATOM | 1343 | C | VAL | 179 | -3.945 | 27.843 | 52.182 | 1.00 23.89 |
| MOTA | 1344 | 0 | VAL | 179 | -4.370 | 27.865 | 51.020 | 1.00 22.84 |
| ATOM | 1345 | N | LEU | 180 | -3.718 | 28.941 | 52.900 | 1.00 25.31 |
| MOTA | 1346 | CA | LEU | 180 | -3.898 | 30.291 | 52.363 | 1.00 27.62 |
| ATOM | 1347 | CB | LEU | 180 | -4.873 | 31.098 | 53.223 | 1.00 29.45 |
| MOTA | 1348 | CG | LEU | 180 | -6.349 | 30.724 | 53.135 | 1.00 32.82 |
| MOTA | 1349 | CD1 | LEU | 180 | -7.138 | 31.542 | 54.147 | 1.00 31.62 |
| MOTA | 1350 | CD2 | LEU | 180 | -6.861 | 30.980 | 51.720 | 1.00 30.67 |
| MOTA | 1351 | С | LEU | 180 | -2.537 | 30.962 | 52.398 | 1.00 27.37 |
| ATOM | 1352 | 0 | LEU | 180 | -1.943 | 31.094 | 53.464 | 1.00 26.56 |
| MOTA | 1353 | N | GLU | 181 | -2.052 | 31.383 | 51.235 | 1.00 28.04 |
| MOTA | 1354 | CA | GLU | 181 | -0.743 | 32.017 | 51.131 | 1.00 30.09 |
| ATOM | 1355 | CB | GLU | 181 | 0.131 | 31.261 | 50.123 | 1.00 30.40 |
| ATOM | 1356 | CG | GLU | 181 | 1.579 | 31.735 | 50.082 | 1.00 33.41 |
| ATOM | 1357 | CD | GLU | 181 | 2.419 | 30.986 | 49.064 | 1.00 35.66 |
| ATOM | 1358 | OE1 | | 181 | 2.297 | 29.747 | 48.986 | 1.00 35.41 |
| ATOM | 1359 | OE2 | GLU | 181 | 3.213 | 31.632 | 48.349 | 1.00 38.36 |
| ATOM | 1360 | C | GLU | 181 | -0.821 | 33.477 | 50.709 | 1.00 30.13 1.00 31.04 |
| ATOM | 1361 | 0 | GLU | 181 | -1.465 | 33.809 | 49.714 51.474 | 1.00 31.04 |
| ATOM | 1362 | N | CYS | 182 | -0.154 | 34.337 35.764 | | 1.00 30.42 |
| ATOM | 1363 | CA | CYS | 182 | -0.097 | 36.026 | 51.195 50.111 | 1.00 31.83 |
| MOTA | 1364 | CB | CYS | 182 182 | 0.946 2.594 | 35.443 | 50.588 | 1.00 36:42 |
| ATOM | 1365 | SG | CYS | 182 | -1.430 | 36.382 | 50.803 | 1.00 30.42 |
| ATOM | 1366 1367 | С 0 | CYS CYS | 182 | -1.683 | 36.677 | 49.632 | 1.00 30.94 |
| ATOM ATOM | 1368 | N | VAL | 183 | -2.273 | 36.580 | 51.807 | 1.00 30.94 |
| ATOM | 1369 | CA | VAL | 183 | -3.587 | 37.165 | 51.614 | 1.00 34.24 |
| ATOM | 1370 | CB | VAL | 183 | -4.674 | 36.054 | 51.575 | 1.00 33.56 |
| ATOM | 1371 | CG1 | | 183 | -4.945 | 35.517 | 52.974 | 1.00 34.62 |
| ATOM | 1372 | CG2 | VAL | 183 | -5.936 | 36.580 | 50.944 | 1.00 35.73 |
| ATOM | 1373 | C | VAL | 183 | -3.846 | 38.118 | 52.786 | 1.00 35.32 |
| ATOM | 1374 | ō | VAL | 183 | -3.400 | 37.870 | 53.909 | 1.00 36.95 |
| ATOM | 1375 | N | PRO | 184 | -4.556 | 39.232 | 52.538 | 1.00 35.89 |
| ATOM | 1376 | CD | PRO | 184 | -5.239 | 39.654 | 51.302 | 1.00 35.39 |
| ATOM | 1377 | CA | PRO | 184 | -4.827 | 40.170 | 53.631 | 1.00 34.72 |
| ATOM | 1378 | CB | PRO | 184 | -5.751 | 41.203 | 52.980 | 1.00 35.50 |
| ATOM | 1379 | CG | PRO | 184 | -6.394 | 40.449 | 51.849 | 1.00 36.10 |
| MOTA | 1380 | С | PRO | 184 | -5.458 | 39.476 | 54.834 | 1.00 33.29 |
| MOTA | 1381 | 0 | PRO | 184 | -6.384 | 38.679 | 54.688 | 1.00 33.08 |
| ATOM | 1382 | N | VAL | 185 | -4.945 | 39.784 | 56.022 | 1.00 33.66 |
| MOTA | 1383 | CA | VAL | 185 | -5.440 | 39.184 | 57.261 | 1.00 33.09 |
| MOTA | 1384 | CB | VAL | 185 | -4.917 | 39.936 | 58.504 | 1.00 33.17 |
| ATOM | 1385 | | VAL | 185 | -5.309 | 39.182 | 59.763 | 1.00 33.65 |
| ATOM | 1386 | CG2 | | 185 | -3.415 | 40.099 | 58.430 | 1.00 31.75 |
| ATOM | 1387 | C | VAL | 185 | -6.960 | 39.165 | 57.338 | 1.00 33.78 |
| MOTA | 1388 | 0 | VAL | 185 | -7.559 | 38.166 | 57.739 | 1.00 33.51 |
| ATOM | 1389 | N | GLU | 186 | -7.577 | 40.282 | 56.968 | 1.00 35.07 |
| ATOM | 1390 | CA | ĢLU | 186 | -9.030 | 40.407 | 56.991 | 1.00 36.33 |
| ATOM | 1391 | CB | GLU | 186 | -9.445 | 41.766 | 56.417 | 1.00 37.40 |
| MOTA | 1392 | CG | GLU | 186 | -8.658 | 42.181 | 55.181 55.508 | 1.00 42.15 1.00 44.18 |
| ATOM | 1393 1394 | CD OE1 | GLU GLU | 186 186 | -7.468 -6.790 | 43.080 42.840 | 56.533 | 1.00 44.18 |
| ATOM ATOM | 1395 | OE2 | | 186 | -7.205 | 44.022 | 54.726 | 1.00 45.83 |
| ATOM | 1396 | C | GLU | 186 | -9.712 | 39.289 | 56.208 | 1.00 35.05 |
| ATOM | 1397 | 0 | GLU | 186 | -10.704 | 38.714 | 56.659 | 1.00 35.03 |
| ATOM | 1398 | N | LEU | 187 | -9.178 | 38.986 | 55.031 | 1.00 34.38 |
| ATOM | 1399 | CA | LEU | 187 | -9.743 | 37.941 | 54.188 | 1.00 33.21 |
| ATOM | 1400 | СВ | LEU | 187 | -9.079 | 37.971 | 52.809 | 1.00 35.04 |
| ATOM | 1401 | CG | LEU | 187 | -9.927 | 37.542 | 51.607 | 1.00 36.74 |
| ATOM | 1402 | | LEU | 187 | -9.075 | 37.607 | 50.351 | 1.00 37.59 |
| ATOM | 1403 | | LEU | 187 | -10.475 | 36.146 | 51.807 | 1.00 36.68 |
| ATOM | 1404 | С | LEU | 187 | -9.533 | 36.577 | 54.836 | 1.00 32.03 |
| MOTA | 1405 | 0 | LEU | 187 | -10.431 | 35.735 | 54.839 | 1.00 30.51 |
| MOTA | 1406 | N | ALA | 188 | -8.340 | 36.364 | 55.386 | 1.00 31.07 |
| ATOM | 1407 | CA | ALA | 188 | -8.012 | 35.102 | 56.039 | 1.00 31.01 |
| MOTA | 1408 | CB | ALA | 188 | -6.576 | 35.138 | 56.554 | 1.00 30.06 |
| ATOM | 1409 | C | ALA | 188 | -8.979 | 34.822 | 57.182 | 1.00 30.77 |
| ATOM | 1410 | 0 | ALA | 188 | -9.345 | 33.673 | 57.424 | 1.00 30.09 |
| ATOM | 1411 | N | LYS | 189 | -9.396 | 35.880 | 57.876 | 1.00 32.19 |
| ATOM | 1412 | CA | LYS | 189 | -10.332 | 35.755 | 58.992 | 1.00 33.17 |
| ATOM | 1413 | CB | LYS | 189 | -10.573 | 37.119 | 59.653 | 1.00 35.50 |
| MOTA | 1414 | CG | LYS | 189 | -9.321 | 37.829 | 60.131 | 1.00 41.20 |

| MOTA | 1415 | CD | LYS | 189 | | -9.644 | 39.151 | 60.826 | 1.00 | 44.52 |
|--------------|--------------|----------|------------|------------|---|--------------------|------------------|------------------|------|----------------|
| MOTA | 1416 | CE | LYS | 189 | | -8.375 | 39.807 | 61.361 | | 46.20 |
| MOTA | 1417 | NZ | LYS | 189 | | -8.623 | 41.120 | 62.025 | | 49.12 |
| MOTA | 1418 | С | LYS | 189 | | -11.672 | 35.201 | 58.520 | | 32.13 |
| MOTA | 1419 | 0 | LYS | 189 | | -12.226 | 34.284 | 59.130 | | 32.62 |
| MOTA | 1420 | N | ARG | 190 | | -12.193 | 35.772 | 57.437 | | 32.40 |
| MOTA | 1421 | CA | ARG | 190 | | -13.478 | 35.343 | 56.887 | | 33.08 |
| MOTA | 1422 | CB | ARG | 190 | | -13.839 | 36.172 | 55.650 | | 34.06 |
| ATOM | 1423 | CG | ARG | 190 | | -14.021 | 37.652 | 55.906 | | 37.30 38.35 |
| ATOM | 1424 1425 | CD | ARG ARG | 190 190 | | -14.906 -14.261 | 38.274 38.346 | 54.834 53.528 | | 38.64 |
| ATOM ATOM | 1425 | NE CZ | ARG | 190 | | -14.920 | 38.343 | 52.373 | | 38.37 |
| ATOM | 1427 | | ARG | 190 | | -16.242 | 38.262 | 52.364 | | 37.74 |
| ATOM | 1428 | NH2 | | 190 | | -14.265 | 38.435 | 51.223 | | 38.25 |
| ATOM | 1429 | C | ARG | 190 | | -13.480 | 33.869 | 56.508 | | 31.06 |
| MOTA | 1430 | 0 | ARG | 190 | | -14.363 | 33.115 | 56.913 | 1.00 | 31.92 |
| ATOM | 1431 | N | ILE | 191 | | -12.488 | 33.466 | 55.723 | 1.00 | 31.60 |
| ATOM | 1432 | CA | ILE | 191 | | -12.391 | 32.081 | 55.283 | 1.00 | 30.50 |
| ATOM | 1433 | CB | ILE | 191 | | -11.197 | 31.887 | 54.322 | | 32.14 |
| ATOM | 1434 | CG2 | ILE | 191 | | -11.045 | 30.412 | 53.965 | | 32.40 |
| MOTA | 1435 | CG1 | ILE | 191 | | -11.415 | 32.724 | 53.057 | | 32.62 |
| ATOM | 1436 | CD1 | ILE | 191 | | -10.227 | 32.763 | 52.116 | | 33.46 |
| ATOM | 1437 | C | ILE | 191 | | -12.245 | 31.133 | 56.466 | | 29.60 |
| ATOM | 1438 | 0 | ILE | 191 | | -12.885 | 30.084 | 56.509 | | 29.78 28.46 |
| MOTA | 1439 | N | THR | 192 | | -11.410 | 31.509 30.673 | 57.428 58.597 | | 28.93 |
| ATOM | 1440 1441 | CA CB | THR THR | 192 192 | | -11.190 -10.100 | 31.269 | 59.514 | | 28.24 |
| MOTA ATOM | 1442 | OG1 | | 192 | | -8.870 | 31.379 | 58.788 | | 28.74 |
| ATOM | 1443 | CG2 | THR | 192 | | -9.878 | 30.380 | 60.723 | 1.00 | 27.20 |
| ATOM | 1444 | C | THR | 192 | | -12.472 | 30.478 | 59.402 | | 29.99 |
| ATOM | 1445 | 0 | THR | 192 | | -12.747 | 29.378 | 59.885 | 1.00 | 28.00 |
| MOTA | 1446 | N | GLU | 193 | | -13.257 | 31.542 | 59.548 | 1.00 | 31.93 |
| ATOM | 1447 | CA | GLU | 193 | | -14.507 | 31.451 | 60.295 | 1.00 | 33.82 |
| MOTA | 1448 | CB | GLU | 193 | | -15.021 | 32.845 | 60.666 | | 36.65 |
| MOTA | 1449 | CG | GLU | 193 | | -14.225 | 33.543 | 61.751 | | 41.54 |
| MOTA | 1450 | CD | GLU | 193 | | -14.789 | 34.912 | 62.097 | | 44.86 |
| MOTA | 1451 | | GLU | 193 | | -14.740 | 35.816 | 61.233 | | 45.51 |
| ATOM | 1452 | | GLU | 193 | | -15.284 | 35.083 | 63.236 | | 47.21 32.10 |
| MOTA | 1453 | C | GLU | 193 | | -15.567 -16.372 | 30.725 29.974 | 59.480 60.023 | | 33.17 |
| MOTA MOTA | 1454 1455 | O N | GLU ALA | 193 194 | ÷ | -15.554 | | 58.172 | | 31.90 |
| ATOM | 1456 | CA | ALA | 194 | | -16.523 | 30.327 | 57.278 | | 30.74 |
| ATOM | 1457 | CB | ALA | 194 | | -16.446 | 30.980 | 55.910 | | 30.76 |
| ATOM | 1458 | C | ALA | 194 | | -16.352 | 28.818 | 57.140 | | 30.69 |
| ATOM | 1459 | 0 | ALA | 194 | | -17.338 | | 57.051 | 1.00 | 30.09 |
| MOTA | 1460 | N | LEU | 195 | | -15.106 | 28.353 | 57.123 | 1.00 | 29.16 |
| MOTA | 1461 | CA | LEU | 195 | | -14.848 | 26.928 | 56.967 | 1.00 | 27.62 |
| ATOM | 1462 | CB | LEU | 195 | | -13.555 | 26.704 | 56.173 | 1.00 | 28.66 |
| MOTA | 1463 | CG | LEU | 195 | | -13.422 | 27.386 | 54.805 | 1.00 | 29.78 |
| MOTA | 1464 | | LEU | 195 | | -12.296 | 26.713 | 54.020 | 1.00 | 28.71 |
| ATOM | 1465 | | LEU | 195 | | -14.723 | 27.288 | 54.034 | | 30.26 |
| ATOM | 1466 | C | LEU | 195 195 | | -14.774 -14.280 | 26.156 26.658 | 58.279 59.290 | | 26.86 26.51 |
| MOTA MOTA | 1467 1468 | O N | LEU ALA | 195 | | -14.280 | 24.931 | 58.247 | 1.00 | 24.22 |
| ATOM | 1469 | N CA | ALA | 196 | | -15.282 | 24.046 | 59.403 | | 24.93 |
| ATOM | 1470 | CB | ALA | 196 | | -16.392 | 23.011 | 59.275 | | 25.42 |
| MOTA | 1471 | Ċ | ALA | 196 | | -13.928 | 23.351 | 59.464 | | 25.63 |
| ATOM | 1472 | Ō | ALA | 196 | | -13.461 | 22.973 | 60.537 | | 24.87 |
| MOTA | 1473 | N | ILE | 197 | | -13.307 | 23.174 | 58.299 | 1.00 | 25.00 |
| MOTA | 1474 | CA | ILE | 197 | | -12.003 | 22.527 | 58.225 | 1.00 | 23.95 |
| MOTA | 1475 | CB | ILE | 197 | | -11.698 | 22.011 | 56.800 | | 22.76 |
| MOTA | 1476 | CG2 | ILE | 197 | | -12.670 | 20.901 | 56.426 | | 21.58 |
| ATOM | 1477 | CG1 | ILE | 197 | | -11.782 | 23.156 | 55.796 | | 22.43 |
| ATOM | 1478 | CD1 | ILE | 197 | | -11.166 | 22.818 | 54.447 | | 24.79 |
| ATOM | 1479 | C | ILE | 197 | | -10.910 | 23.505 | 58.628 | | 24.38 |
| ATOM | 1480 | O N | ILE | 197 | | -11.011 -9.845 | 24.709 23.001 | 58.381 59.260 | | 24.17 24.33 |
| ATOM ATOM | 1481 | N | PRO | 198 198 | | -9.845 -9.578 | 23.001 | 59.260 | | 23.43 |
| ATOM ATOM | 1482 1483 | CD CA | PRO PRO | 198 | | -8.768 | 23.903 | 59.668 | | 24.80 |
| ATOM | 1484 | CB | PRO | 198 | | -7.840 | 22.994 | 60.482 | | 24.52 |
| ATOM | 1485 | CG | PRO | 198 | | -8.104 | 21.638 | 59.926 | | 26.07 |
| ATOM | 1486 | C | PRO | 198 | | -8.070 | 24.579 | 58.489 | | 23.71 |
| ATOM | 1487 | ŏ | PRO | 198 | | -7.840 | 23.965 | 57.445 | | 24.75 |
| MOTA | 1488 | N | VAL | 199 | | -7.765 | 25.859 | 58.659 | | 22.66 |
| MOTA | 1489 | CA | VAL | 199 | | -7.090 | 26.628 | 57.633 | | 21.26 |
| MOTA | 1490 | CB | VAL | 199 | | | 27.952 | | | 21.86 |
| MOTA | 1491 | CG1 | VAL | 199 | | -7.104 | 28.753 | 56.286 | 1.00 | 21.68 |

| ATOM | 1492 | CG2 VAL | 199 | -9.261 | 27.651 | 56.881 | 1.00 23.56 |
|------|------|------------|-----|--------|--------|--------|------------|
| ATOM | 1493 | C VAL | 199 | -5.677 | 26.948 | 58.113 | 1.00 22.90 |
| | | | 199 | -5.489 | 27.514 | 59.191 | 1.00 21.18 |
| MOTA | 1494 | | | | | | |
| ATOM | 1495 | N ILE | 200 | -4.689 | 26.568 | 57.311 | 1.00 21.02 |
| MOTA | 1496 | CA ILE | 200 | -3.286 | 26.799 | 57.633 | 1.00 20.82 |
| ATOM | 1497 | CB ILE | 200 | -2.425 | 25.579 | 57.265 | 1.00 22.17 |
| MOTA | 1498 | CG2 ILE | 200 | -0.956 | 25.857 | 57.584 | 1.00 21.54 |
| | | CG1 ILE | 200 | -2.925 | 24.346 | 58.015 | 1.00 21.31 |
| MOTA | 1499 | | | | | | |
| MOTA | 1500 | CD1 ILE | 200 | -2.202 | 23.066 | 57.627 | 1.00 26.13 |
| MOTA | 1501 | C ILE | 200 | -2.800 | 27.984 | 56.821 | 1.00 21.27 |
| ATOM | 1502 | O ILE | 200 | -2.820 | 27.952 | 55.590 | 1.00 19.70 |
| ATOM | 1503 | N GLY | 201 | -2.344 | 29.025 | 57.505 | 1.00 21.83 |
| ATOM | 1504 | CA GLY | 201 | -1.883 | 30.199 | 56.791 | 1.00 21.11 |
| | | | | | | | |
| MOTA | 1505 | C GLY | 201 | -0.382 | 30.376 | 56.722 | 1.00 21.20 |
| MOTA | 1506 | O GLY | 201 | 0.360 | 29.915 | 57.586 | 1.00 20.91 |
| ATOM | 1507 | N ILE | 202 | 0.053 | 31.035 | 55.656 | 1.00 20.88 |
| ATOM | 1508 | CA ILE | 202 | 1.449 | 31.357 | 55.434 | 1.00 23.63 |
| ATOM | 1509 | CB ILE | 202 | 2.135 | 30.374 | 54.442 | 1.00 25.53 |
| | 1510 | CG2 ILE | 202 | 1.199 | 30.026 | 53.295 | 1.00 25.11 |
| ATOM | | | | | | | |
| MOTA | 1511 | CG1 ILE | 202 | 3.431 | 30.991 | 53.922 | 1.00 26.37 |
| ATOM | 1512 | CD1 ILE | 202 | 4.537 | 31.025 | 54.938 | 1.00 25.90 |
| ATOM | 1513 | C ILE | 202 | 1.401 | 32.754 | 54.827 | 1.00 23.67 |
| ATOM | 1514 | O ILE | 202 | 1.098 | 32.921 | 53.647 | 1.00 24.24 |
| ATOM | 1515 | N GLY | 203 | 1.672 | 33.760 | 55.649 | 1.00 24.85 |
| | | | | | | | |
| MOTA | 1516 | CA GLY | 203 | 1.615 | 35.130 | 55.177 | 1.00 24.91 |
| MOTA | 1517 | C GLY | 203 | 0.167 | 35.580 | 55.162 | 1.00 24.72 |
| MOTA | 1518 | O GLY | 203 | -0.222 | 36.447 | 54.378 | 1.00 26.70 |
| ATOM | 1519 | | 204 | -0.635 | 34.981 | 56.037 | 1.00 24.39 |
| | 1520 | | 204 | -2.054 | 35.308 | 56.132 | 1.00 25.25 |
| MOTA | | | | | | | |
| MOTA | 1521 | CB ALA | 204 | -2.889 | 34.113 | 55.704 | 1.00 25.27 |
| ATOM | 1522 | C ALA | 204 | -2.467 | 35.745 | 57.538 | 1.00 25.30 |
| ATOM | 1523 | O ALA | 204 | 3.648 | 35.701 | 57.885 | 1.00 26.25 |
| ATOM | 1524 | N GLY | 205 | -1.495 | 36.155 | 58.346 | 1.00 26.07 |
| | | | 205 | -1.798 | 36.597 | 59.699 | 1.00 25.17 |
| ATOM | 1525 | CA GLY | | | | | |
| MOTA | 1526 | C GLY | 205 | -1.952 | 35.459 | 60.688 | 1.00 25.65 |
| ATOM | 1527 | O GLY | 205 | -1.853 | 34.294 | 60.316 | 1.00 24.90 |
| ATOM | 1528 | N ASN | 206 | -2.195 | 35.791 | 61.952 | 1.00 24.53 |
| ATOM | 1529 | CA ASN | 206 | -2.350 | 34.772 | 62.983 | 1.00 24.06 |
| | 1530 | | 206 | -1.739 | 35.250 | 64.298 | 1.00 25.67 |
| ATOM | | | | | | | |
| MOTA | 1531 | CG ASN | 206 | -2.512 | 36.405 | 64.915 | 1.00 27.21 |
| MOTA | 1532 | OD1 ASN | 206 | -2.316 | 36.744 | 66.081 | 1.00 27.76 |
| ATOM | 1533 | ND2 ASN | 206 | -3.393 | 37.016 | 64.131 | 1.00 24.74 |
| ATOM | 1534 | C ASN | 206 | -3.805 | 34.407 | 63.230 | 1.00 22.53 |
| | 1535 | | 206 | -4.127 | 33.788 | 64.246 | 1.00 21.69 |
| ATOM | | | | | | | |
| MOTA | 1536 | N VAL | 207 | -4.680 | 34.786 | 62.305 | 1.00 21.94 |
| ATOM | 1537 | CA VAL | 207 | -6.098 | 34.496 | 62.446 | 1.00 23.84 |
| ATOM | 1538 | CB VAL | 207 | -6.953 | 35.513 | 61.668 | 1.00 26.20 |
| ATOM | 1539 | CG1 VAL | 207 | -8.423 | 35.336 | 62.037 | 1.00 29.08 |
| ATOM | 1540 | CG2 VAL | 207 | -6.488 | 36.925 | 61.981 | 1.00 27.68 |
| | 1541 | | 207 | -6.453 | 33.091 | 61.965 | 1.00 24.32 |
| MOTA | | C VAL | | | | | |
| ATOM | 1542 | O VAL | 207 | -7.563 | 32.600 | 62.203 | 1.00 23.30 |
| MOTA | 1543 | N THR | 208 | -5.513 | 32.431 | 61.297 | 1.00 23.32 |
| ATOM | 1544 | CA THR | 208 | -5.779 | 31.086 | 60.811 | 1.00 23.51 |
| ATOM | 1545 | CB THR | 208 | -4.840 | 30.708 | 59.643 | 1.00 23.12 |
| ATOM | 1546 | OG1 THR | 208 | -3.481 | 30.977 | 60.008 | 1.00 21.10 |
| | | | | | | 58.402 | 1.00 21.10 |
| MOTA | 1547 | CG2 THR | 208 | -5.198 | 31.502 | | |
| MOTA | 1548 | C THR | 208 | -5.663 | 30.053 | 61.919 | 1.00 24.29 |
| MOTA | 1549 | O THR | 208 | -5.129 | 30.331 | 62.995 | 1.00 24.25 |
| ATOM | 1550 | N ASP | 209 | -6.185 | 28.861 | 61.657 | 1.00 22.58 |
| MOTA | 1551 | CA ASP | 209 | -6.164 | 27.788 | 62.642 | 1.00 22.69 |
| | | A. Carrier | 209 | -7.091 | 26.665 | 62.194 | 1.00 22.67 |
| ATOM | 1552 | CB ASP | | | | | |
| MOTA | 1553 | CG ASP | 209 | -8.501 | 27.146 | 61.961 | 1.00 25.87 |
| MOTA | 1554 | OD1 ASP | 209 | -9.130 | 27.621 | 62.931 | 1.00 23.71 |
| MOTA | 1555 | OD2 ASP | 209 | -8.980 | 27.056 | 60.808 | 1.00 24.21 |
| ATOM | 1556 | C ASP | 209 | -4.764 | 27.244 | 62.830 | 1.00 21.49 |
| ATOM | 1557 | O ASP | 209 | -4.451 | 26.657 | 63.863 | 1.00 21.81 |
| | | | | -3.928 | 27.444 | 61.819 | 1.00 21.84 |
| MOTA | 1558 | N GLY | 210 | | | | |
| MOTA | 1559 | CA GLY | 210 | -2.569 | 26.956 | 61.891 | 1.00 20.56 |
| MOTA | 1560 | C GLY | 210 | -1.623 | 27.775 | 61.043 | 1.00 20.58 |
| MOTA | 1561 | O GLY | 210 | -2.049 | 28.651 | 60.287 | 1.00 21.05 |
| ATOM | 1562 | N GLN | 211 | -0.332 | 27.473 | 61.156 | 1.00 20.83 |
| ATOM | 1563 | | 211 | 0.699 | 28.192 | 60.424 | 1.00 21.52 |
| | | CA GLN | | | | | |
| MOTA | 1564 | CB GLN | 211 | 1.459 | 29.119 | 61.379 | 1.00 22.07 |
| ATOM | 1565 | CG GLN | 211 | 0.626 | 30.239 | 61.993 | 1.00 19.78 |
| ATOM | 1566 | CD GLN | 211 | 0.135 | 31.229 | 60.960 | 1.00 21.63 |
| MOTA | 1567 | OE1 GLN | 211 | 0.895 | 31.663 | 60.093 | 1.00 23.63 |
| ATOM | 1568 | NE2 GLN | 211 | -1.139 | 31.608 | 61.055 | 1.00 21.71 |
| 011 | 1300 | TILD CITIN | | | | | |
| | | | | | | | |

| ATOM | 1569 | С | GLN | 211 | 1.701 | 27.250 | 59.761 | 1.00 21.50 |
|--------------|--------------|------------|------------|------------|------------------|------------------|------------------|--------------------------|
| MOTA | 1570 | 0 | GLN | 211 | 1.886 | 26.117 | 60.199 | 1.00 20.81 |
| MOTA | 1571 | N | ILE | 212 | 2.344 | 27.724 | 58.700 | 1.00 22.48 |
| ATOM | 1572 | CA | ILE | 212 | 3.351 | 26.921 | 58.023 | 1.00 26.35 |
| MOTA | 1573 | CB | ILE | 212 | 2.755 | 26.171 | 56.799 | 1.00 28.17 |
| ATOM | 1574 | CG2 | ILE | 212 | 2.484 | 27.139 | 55.660 | 1.00 29.37 |
| ATOM | 1575 | CG1 | ILE | 212 | 3.725 | 25.075 | 56.344 | 1.00 29.11 |
| ATOM | 1576 | CD1 | ILE | 212 | 3.081 | 24.015 | 55.457 | 1.00 31.12 |
| ATOM | 1577 | С | ILE | 212 | 4.494 | 27.829 | 57.588 | 1.00 28.11 |
| ATOM | 1578 | 0 | ILE | 212 | 4.287 | 29.011 | 57.319 | 1.00 29.09 |
| ATOM | 1579 | N | LEU | 213 | 5.706 | 27.287 | 57.556 | 1.00 29.45 |
| ATOM | 1580 | CA | LEU | 213 | 6.870 | 28.062 | 57.135 | 1.00 31.99 |
| MOTA | 1581 | CB | LEU | 213 | 7.432 | 28.880 | 58.300 | 1.00 33.40 |
| ATOM | 1582 | CG | LEU | 213 | 7.351 | 30.415 | 58.241 | 1.00 33.83 |
| MOTA | 1583 | CD1 | LEU | 213 | 8.119 | 30.972 | 59.435 | 1.00 32.93 |
| MOTA | 1584 | CD2 | LEU | 213 | 7.941 | 30.952 | 56.936 | 1.00 31.79 |
| ATOM | 1585 | С | LEU | 213 | 7.970 | 27.159 | 56.602 | 1.00 32.15 |
| MOTA | 1586 | 0 | LEU | 213 | 8.143 | 26.033 | 57.076 | 1.00 31.38 |
| MOTA | 1587 | N | VAL | 214 | 8.699 | 27.656 | 55.607 | 1.00 31.01 |
| MOTA | 1588 | CA | VAL | 214 | 9.808 | 26.913 | 55.025 | 1.00 30.31 |
| MOTA | 1589 | CB | VAL | 214 | 10.300 | 27.550 | 53.695 | 1.00 31.87 |
| ATOM | 1590 | CG1 | VAL | 214 | 11.516 | 26.796 | 53.174 | 1.00 32.34 |
| MOTA | 1591 | CG2 | VAL | 214 | 9.188 | 27.505 | 52.659 | 1.00 33.39 |
| MOTA | 1592 | C | VAL | 214 | 10.923 | 26.976 | 56.060 | 1.00 28.15 |
| MOTA | 1593 | 0 | VAL | 214 | 11.440 | 28.050 | 56.362 | 1.00 28.96 |
| MOTA | 1594 | N | MET | 215 | 11.268 | 25.820 | 56.614 | 1.00 25.80 |
| MOTA | 1595 | CA | MET | 215 | 12.299 | 25.727 | 57.632 | 1.00 24.04 |
| ATOM | 1596 | CB | MET | 215 | 12.617 | 24.254 | 57.927 | 1.00 21.67 |
| MOTA | 1597 | CG | MET | 215 | 13.046 | 23.449 | 56.708 | 1.00 21.44 |
| MOTA | 1598 | SD | MET | 215 | 14.311 | 22.218 | 57.084 | 1.00 19.28 |
| MOTA. | 1599 | CE | MET | 215 | 15.756 | 23.248 | 56.942 | 1.00 20.16 |
| ATOM | 1600 | С | MET | 215 | 13.575 | 26.465 | 57.253 | 1.00 23.77 |
| MOTA | 1601 | 0 | MET | 215 | 14.253 | 27.025 | 58.114 | 1.00 24.19 |
| MOTA | 1602 | N | HIS | 216 | 13.901 | 26.489 | 55.966 | 1.00 23.61 |
| MOTA | 1603 | CA | HIS | 216 | 15.122 | 27.163 | 55.520 | 1.00 25.02 |
| MOTA | 1604 | CB | HIS | 216 | 15.342 | 26.890 | 54.035 | 1.00 25.17 |
| MOTA | 1605 | CG | HIS | 216 | 15.707 | 25.468 | 53.751 | 1.00 25.07 |
| ATOM | 1606 | CD2 | | 216 | 14.939 | 24.360 | 53.621 | 1.00 22.61 |
| ATOM | 1607 | ND1 | | 216 | 17.014 | 25.039 | 53.656 | 1.00 24.95 |
| ATOM | 1608 | CE1 | | 216 | 17.035 | 23.730 | 53.479 | 1.00 23.43 |
| ATOM | 1609 | NE2 | | 216 | 15.788 | 23.294 | 53.455 | 1.00 26.42 |
| ATOM | 1610 | C | HIS | 216 | 15.132 | 28.659 | 55.812 | 1.00 26.05 |
| ATOM | 1611 | 0 | HIS | 216 | 16.195 | 29.277 | 55.872 | 1.00 25.85 |
| ATOM | 1612 | N | ASP | 217 | 13.949 | 29.238 | 56.000 | 1.00 27.68 |
| MOTA | 1613 | CA | ASP | 217 | 13.848 | 30.661 | 56.321 | 1.00 31.25 |
| ATOM | 1614 | CB | ASP | 217 | 12.576 | 31.271 31.406 | 55.713 | 1.00 33.06 |
| ATOM | 1615 | CG CD1 | ASP | 217 217 | 12.653 | | 54.200 53.700 | 1.00 35.27 1.00 36.27 |
| ATOM ATOM | 1616 | OD1 OD2 | | 217 | 13.623 11.735 | 32.016 30.916 | 53.507 | 1.00 30.27 |
| ATOM | 1617 1618 | C | ASP ASP | 217 | 13.827 | 30.825 | 57.845 | 1.00 37.03 |
| ATOM | 1619 | 0 | ASP | 217 | 14.353 | 31.803 | 58.394 | 1.00 31.02 |
| | 1620 | N | ALA | 217 | 13.225 | 29.853 | 58.524 | 1.00 32.33 |
| MOTA | 1621 | CA | ALA | 218 | 13.121 | 29.882 | 59.981 | 1.00 30.59 |
| ATOM | 1622 | CB | ALA | 218 | 12.208 | 28.761 | 60.451 | 1.00 30.22 |
| ATOM | 1623 | C | ALA | 218 | 14.471 | 29.783 | 60.689 | 1.00 31.33 |
| ATOM | 1624 | ō | ALA | 218 | 14.593 | 30.180 | 61.851 | 1.00 31.23 |
| ATOM | 1625 | N | PHE | 219 | 15.482 | 29.267 | 59.992 | 1.00 30.28 |
| ATOM | 1626 | CA | PHE | 219 | 16.804 | 29.117 | 60.589 | 1.00 29.83 |
| ATOM | 1627 | CB | PHE | 219 | 17.202 | 27.640 | 60.598 | 1.00 29.92 |
| ATOM | 1628 | CG | PHE | 219 | 16.148 | 26.736 | 61.177 | 1.00 30.71 |
| ATOM | 1629 | CD1 | | 219 | 15.529 | 27.052 | 62.385 | 1.00 31.14 |
| ATOM | 1630 | | PHE | 219 | 15.781 | 25.562 | 60.524 | 1.00 31.43 |
| ATOM | 1631 | CE1 | | 219 | 14.562 | 26.213 | 62.935 | 1.00 31.73 |
| ATOM | 1632 | CE2 | | 219 | 14.811 | 24.714 | 61.067 | 1.00 32.41 |
| ATOM | 1633 | CZ | PHE | 219 | 14.202 | 25.041 | 62.275 | 1.00 31.77 |
| ATOM | 1634 | С | PHE | 219 | 17.881 | 29.943 | 59.899 | 1.00 29.17 |
| MOTA | 1635 | o | PHE | 219 | 19.069 | 29.621 | 59.968 | 1.00 29.21 |
| ATOM | 1636 | N | GLY | 220 | 17.458 | 31.014 | 59.237 | 1.00 29.74 |
| MOTA | 1637 | CA | GLY | 220 | 18.390 | 31.889 | 58.550 | 1.00 29.75 |
| ATOM | 1638 | C | GLY | 220 | 19.357 | 31.185 | 57.621 | 1.00 30.84 |
| ATOM | 1639 | 0 | GLY | 220 | 20.507 | 31.601 | 57.485 | 1.00 30.29 |
| ATOM | 1640 | N | ILE | 221 | 18.900 | 30.120 | 56.973 | 1.00 30.94 |
| ATOM | 1641 | CA | ILE | 221 | 19.754 | 29.380 | 56.053 | 1.00 30.23 |
| ATOM | 1642 | CB | ILE | 221 | 19.270 | 27.930 | 55.896 | 1.00 28.54 |
| ATOM | 1643 | CG2 | ILE | 221 | 20.167 | 27.187 | 54.908 | 1.00 26.85 |
| MOTA | 1644 | CG1 | ILE | 221 | 19.288 | 27.239 | 57.263 | 1.00 27.41 |
| MOTA | 1645 | CD1 | ILE | 221 | 18.654 | 25.879 | 57.279 | 1.00 26.63 |
| | | | | | | | | |

| ATOM | 1646 | С | ILE | 221 | 19.759 | 30.060 | 54.691 | 1.00 31.63 |
|------|------|-----|-----|-------|--------|--------|--------|------------|
| ATOM | 1647 | 0 | ILE | 221 | 20.799 | 30.178 | 54.041 | 1.00 30.47 |
| | | | | | | | | |
| ATOM | 1648 | N | THR | 222 | 18.590 | 30.528 | 54.275 | 1.00 33.36 |
| ATOM | 1649 | CA | THR | 222 | 18.453 | 31.193 | 52.989 | 1.00 37.25 |
| ATOM | 1650 | CB | THR | 222 | 16.981 | 31.241 | 52.555 | 1.00 36.65 |
| ATOM | 1651 | OG1 | THR | 222 | 16.249 | 32.088 | 53.448 | 1.00 39.18 |
| ATOM | 1652 | CG2 | THR | 222 | 16.375 | 29.851 | 52.594 | 1.00 35.68 |
| | | | | | | | | |
| ATOM | 1653 | C | THR | 222 | 18.995 | 32.616 | 53.029 | 1.00 39.66 |
| ATOM | 1654 | 0 | THR | 222 | 18.770 | 33.345 | 53.993 | 1.00 39.16 |
| MOTA | 1655 | N | GLY | 223 | 19.713 | 32.990 | 51.970 | 1.00 43.16 |
| MOTA | 1656 | CA | GLY | 223 | 20.292 | 34.320 | 51.848 | 1.00 47.53 |
| MOTA | 1657 | С | GLY | 223 | 20.326 | 35.168 | 53.105 | 1.00 50.12 |
| | | | | | | | | |
| MOTA | 1658 | 0 | GLY | 223 | 20.927 | 34.786 | 54.110 | |
| MOTA | 1659 | N | GLY | 224 | 19.680 | 36.327 | 53.052 | 1.00 51.89 |
| MOTA | 1660 | CA | GLY | 224 | 19.663 | 37.202 | 54.207 | 1.00 54.05 |
| ATOM | 1661 | С | GLY | 224 | 18.324 | 37.871 | 54.422 | 1.00 56.18 |
| ATOM | 1662 | 0 | GLY | 224 | 17.767 | 37.824 | 55.520 | 1.00 56.72 |
| | | | | 225 | 17.802 | 38.495 | 53.371 | 1.00 57.60 |
| MOTA | 1663 | N | HIS | | | | | |
| MOTA | 1664 | CA | HIS | 225 | 16.520 | 39.185 | 53.453 | 1.00 58.83 |
| MOTA | 1665 | CB | HIS | 225 | 16.487 | 40.359 | 52.470 | 1.00 61.50 |
| ATOM | 1666 | CG | HIS | 225 | 17.419 | 41.475 | 52.828 | 1.00 63.93 |
| ATOM | 1667 | CD2 | HIS | 225 | 18.446 | 42.036 | 52.146 | 1.00 65.25 |
| ATOM | 1668 | | HIS | 225 | 17.338 | 42.155 | 54.025 | 1.00 65.20 |
| | | | | | | | | |
| MOTA | 1669 | CE1 | | 225 | 18.275 | 43.087 | 54.063 | 1.00 65.92 |
| ATOM | 1670 | | HIS | 225 | 18.960 | 43.036 | 52.935 | 1.00 66.01 |
| ATOM | 1671 | C | HIS | 225 | 15.340 | 38.257 | 53.183 | 1.00 57.89 |
| ATOM | 1672 | 0 | HIS | 225 | 14.797 | 38.234 | 52.079 | 1.00 58.08 |
| ATOM | 1673 | N | ILE | 226 | 14.947 | 37.497 | 54.201 | 1.00 56.71 |
| | | | | | | | | |
| ATOM | 1674 | CA | ILE | 226 | 13.825 | 36.573 | 54.080 | 1.00 55.07 |
| MOTA | 1675 | CB | ILE | 226 | 13.651 | 35.740 | 55.367 | 1.00 55.20 |
| MOTA | 1676 | CG2 | ILE | 226 | 14.888 | 34.885 | 55.601 | 1.00 54.98 |
| MOTA | 1677 | CG1 | ILE | 226 | 13.400 | 36.668 | 56.558 | 1.00 54.81 |
| ATOM | 1678 | CD1 | ILE | 226 | 13.109 | 35.942 | 57.852 | 1.00 54.53 |
| ATOM | 1679 | C | ILE | 226 | 12.541 | 37.359 | 53.820 | 1.00 53.36 |
| ATOM | 1680 | ō | ILE | 226 | 12.499 | 38.576 | 54.020 | 1.00 54.02 |
| | | | | | | | | |
| MOTA | 1681 | N | PRO | 227 | 11.473 | 36.674 | 53.377 | 1.00 50.99 |
| ATOM | 1682 | CD | PRO | 227 | 11.336 | 35.223 | 53.161 | 1.00 49.98 |
| MOTA | 1683 | CA | PRO | 227 | 10.206 | 37.361 | 53.104 | 1.00 48.87 |
| ATOM | 1684 | CB | PRO | 227 | 9.319 | 36.242 | 52.564 | 1.00 48.89 |
| ATOM | 1685 | CG | PRO | 227 | 9.847 | 35.031 | 53.259 | 1.00 49.85 |
| ATOM | 1686 | С | PRO | 227 | 9.615 | 38.045 | 54.336 | 1.00 46.39 |
| ATOM | 1687 | 0 | PRO | 227 | 9.860 | 37.626 | 55.465 | 1.00 46.32 |
| ATOM | 1688 | N | LYS | 228 | 8.839 | 39.101 | 54.108 | 1.00 44.27 |
| MOTA | 1689 | CA | | 228 | 8.222 | 39.850 | 55.195 | 1.00 41.95 |
| | | | LYS | | | | | |
| ATOM | 1690 | CB | LYS | 228 | 7.360 | 40.992 | 54.648 | 1.00 43.42 |
| MOTA | 1691 | CG | LYS | 228 | 8.139 | 42.134 | 54.016 | 1.00 47.18 |
| MOTA | 1692 | CD | LYS | 228 | 8.750 | 41.736 | 52.678 | 1.00 49.90 |
| ATOM | 1693 | CE | LYS | 228 | 9.498 | 42.906 | 52.048 | 1.00 51.00 |
| ATOM | 1694 | NZ | LYS | 228 | 10.007 | 42.601 | 50.679 | 1.00 51.75 |
| ATOM | 1695 | C | LYS | 228 | 7.367 | 38.987 | 56.110 | 1.00 39.05 |
| | | | | | | | | 1.00 39.22 |
| ATOM | 1696 | 0 | LYS | 228 | 7.232 | 39.278 | 57.297 | |
| ATOM | 1697 | N | PHE | 229 | 6.787 | 37.927 | 55.561 | 1.00 35.73 |
| ATOM | 1698 | CA | PHE | 229 | 5.935 | 37.052 | 56.352 | 1.00 31.21 |
| ATOM | 1699 | CB | PHE | 229 | 4.883 | 36.397 | 55.453 | 1.00 32.42 |
| ATOM | 1700 | CG | PHE | 229 | 5.460 | 35.543 | 54.360 | 1.00 32.78 |
| ATOM | 1701 | CD1 | PHE | 229 | 5.908 | 34.253 | 54.625 | 1.00 32.94 |
| ATOM | 1702 | CD2 | PHE | 229 | 5.554 | 36.030 | 53.060 | 1.00 34.15 |
| ATOM | 1703 | CE1 | PHE | 229 | 6.442 | 33.457 | 53.606 | 1.00 32.72 |
| | 1703 | CE2 | | | 6.086 | 35.246 | 52.034 | 1.00 32.72 |
| АТОМ | | | PHE | 229 | | | | |
| ATOM | 1705 | CZ | PHE | 229 . | 6.529 | 33.958 | 52.309 | 1.00 33.05 |
| MOTA | 1706 | С | PHE | 229 | 6.707 | 35.985 | 57.116 | 1.00 28.23 |
| ATOM | 1707 | 0 | PHE | 229 | 6.126 | 35.262 | 57.921 | 1.00 28.17 |
| MOTA | 1708 | N | ALA | 230 | 8.013 | 35.900 | 56.876 | 1.00 26.34 |
| ATOM | 1709 | CA | ALA | 230 | 8.848 | 34.907 | 57.544 | 1.00 24.97 |
| ATOM | 1710 | ĊВ | ALA | 230 | 9.833 | 34.304 | 56.552 | 1.00 26.85 |
| ATOM | 1711 | C | ALA | 230 | 9.605 | 35.484 | 58.734 | 1.00 26.01 |
| ATOM | 1712 | 0 | ALA | 230 | 9.743 | 36.700 | 58.865 | 1.00 25.21 |
| | | | | | | | | |
| ATOM | 1713 | N | LYS | 231 | 10.090 | 34.596 | 59.600 | 1.00 24.27 |
| MOTA | 1714 | CA | LYS | 231 | 10.838 | 34.999 | 60.786 | 1.00 24.53 |
| MOTA | 1715 | CB | LYS | 231 | 9.898 | 35.149 | 61.989 | 1.00 25.49 |
| ATOM | 1716 | CG | LYS | 231 | 10.609 | 35.476 | 63.295 | 1.00 25.37 |
| ATOM | 1717 | CD | LYS | 231 | 9.634 | 35.596 | 64.455 | 1.00 28.18 |
| ATOM | 1718 | CE | LYS | 231 | 10.372 | 35.784 | 65.780 | 1.00 29.49 |
| ATOM | 1719 | NZ | LYS | 231 | 9.434 | 35.995 | 66.923 | 1.00 29.09 |
| ATOM | 1720 | C | LYS | 231 | 11.919 | 33.977 | 61.118 | 1.00 23.25 |
| | | | | | | 32.775 | 61.097 | 1.00 20.91 |
| ATOM | 1721 | 0 | LYS | 231 | 11.674 | | | |
| MOTA | 1722 | N | ASN | 232 | 13.115 | 34.470 | 61.419 | 1.00 22.11 |
| | | | | | | | | |

| ATOM | 1723 | CA | ASN | 232 | 14.238 | 33.617 | 61.775 | 1.00 22.68 |
|--------------|------|--------|------------|-----|--------|--------|--------|------------|
| ATOM | 1724 | CB | ASN | 232 | 15.550 | 34.325 | 61.427 | 1.00 22.74 |
| ATOM | 1725 | CG | ASN | 232 | 16.770 | 33.476 | 61.711 | 1.00 22.28 |
| ATOM | 1726 | | ASN | 232 | 16.710 | 32.519 | 62.477 | 1.00 22.05 |
| ATOM | 1727 | | ASN | 232 | 17.897 | 33.839 | 61.103 | 1.00 21.01 |
| ATOM | 1728 | C | ASN | 232 | 14.157 | 33.363 | 63.283 | 1.00 22.41 |
| ATOM | 1729 | ō | ASN | 232 | 14.442 | 34.256 | 64.083 | 1.00 22.40 |
| ATOM | 1730 | N | PHE | 233 | 13.754 | 32.158 | 63.670 | 1.00 20.06 |
| ATOM | 1731 | CA | PHE | 233 | 13.640 | 31.816 | 65.083 | 1.00 20.00 |
| ATOM | 1732 | CB | PHE | 233 | 12.623 | 30.692 | 65.284 | 1.00 20.88 |
| | 1733 | CG | PHE | 233 | 11.193 | 31.121 | 65.109 | 1.00 20.63 |
| ATOM | 1734 | | PHE | 233 | 10.614 | 31.161 | 63.849 | 1.00 21.32 |
| ATOM ATOM | 1735 | | PHE | 233 | 10.428 | 31.498 | 66.210 | 1.00 20.85 |
| | 1736 | | PHE | 233 | 9.289 | 31.566 | 63.678 | 1.00 21.06 |
| ATOM | 1737 | CE2 | PHE . | 233 | 9.102 | 31.905 | 66.053 | 1.00 21.00 |
| ATOM | 1738 | CZ | PHE | 233 | 8.536 | 31.940 | 64.783 | 1.00 21.27 |
| MOTA | 1739 | | | 233 | 14.973 | 31.400 | 65.698 | 1.00 13.83 |
| ATOM | | C O | PHE PHE | 233 | 15.130 | 31.398 | 66.921 | 1.00 22.96 |
| ATOM | 1740 | | | 234 | 15.130 | 31.033 | 64.852 | 1.00 22.02 |
| ATOM | 1741 | N | LEU | | 17.242 | | | |
| ATOM | 1742 | CA | LEU | 234 | | 30.622 | 65.328 | |
| MOTA | 1743 | CB | LEU | 234 | 18.008 | 29.894 | 64.219 | 1.00 23.62 |
| ATOM | 1744 | CG | LEU | 234 | 19.465 | 29.538 | 64.524 | 1.00 22.78 |
| ATOM | 1745 | | LEU | 234 | 19.527 | 28.580 | 65.701 | 1.00 21.54 |
| ATOM | 1746 | | LEU | 234 | 20.112 | 28.923 | 63.292 | 1.00 25.26 |
| MOTA | 1747 | C | LEU | 234 | 18.045 | 31.838 | 65.773 | 1.00 26.95 |
| ATOM | 1748 | 0 | LEU | 234 | 18.727 | 31.801 | 66.796 | 1.00 25.49 |
| MOTA | 1749 | N | ALA | 235 | 17.958 | 32.911 | 64.996 | 1.00 30.52 |
| MOTA | 1750 | CA | ALA | 235 | 18.681 | 34.138 | 65.302 | 1.00 36.40 |
| MOTA | 1751 | CB | ALA | 235 | 18.274 | 35.239 | 64.331 | 1.00 37.16 |
| ATOM | 1752 | С | ALA | 235 | 18.417 | 34.578 | 66.736 | 1.00 40.32 |
| ATOM | 1753 | 0 | ALA | 235 | 19.337 | 34.973 | 67.454 | 1.00 40.96 |
| ATOM | 1754 | N | GLU | 236 | 17.154 | 34.501 | 67.145 | 1.00 43.98 |
| MOTA | 1755 | CA | GLU | 236 | 16.750 | 34.881 | 68.497 | 1.00 47.59 |
| MOTA | 1756 | CB | GLU | 236 | 15.280 | 34.514 | 68.730 | 1.00 48.96 |
| MOTA | 1757 | CG | GLU | 236 | 14.320 | 34.967 | 67.632 | 1.00 51.28 |
| MOTA | 1758 | CD | GLU | 236 | 14.177 | 36.477 | 67.544 | 1.00 52.90 |
| MOTA | 1759 | OE1 | | 236 | 15.174 | 37.159 | 67.224 | 1.00 53.61 |
| MOTA | 1760 | OE2 | GLU | 236 | 13.063 | 36.984 | 67.798 | 1.00 53.70 |
| MOTA | 1761 | С | GLU | 236 | 17.625 | 34.138 | 69.502 | 1.00 48.66 |
| MOTA | 1762 | 0 | GLU | 236 | 18.234 | 34.748 | 70.380 | 1.00 49.42 |
| MOTA | 1763 | N | THR | 237 | 17.681 | 32.817 | 69.355 | 1.00 49.40 |
| MOTA | 1764 | CA | THR | 237 | 18.475 | 31.967 | 70.235 | 1.00 49.62 |
| ATOM | 1765 | CB | THR | 237 | 17.668 | 30.713 | 70.667 | 1.00 50.79 |
| MOTA | 1766 | OG1 | | 237 | 18.464 | 29.900 | 71.542 | 1.00 52.05 |
| MOTA | 1767 | CG2 | THR | 237 | 17.247 | 29.894 | 69.452 | 1.00 51.76 |
| MOTA | 1768 | С | THR | 237 | 19.772 | 31.529 | 69.548 | 1.00 48.44 |
| ATOM | 1769 | 0 | THR | 237 | 20.349 | 32.278 | 68.759 | 1.00 49.89 |
| MOTA | 1770 | N | GLY | 238 | 20.234 | 30.323 | 69.858 | 1.00 46.44 |
| ATOM | 1771 | CA | GLY | 238 | 21.451 | 29.819 | 69.248 | 1.00 42.67 |
| MOTA | 1772 | С | GLY | 238 | 21.379 | 28.318 | 69.059 | 1.00 41.05 |
| MOTA | 1773 | 0 | GLY | 238 | 22.385 | 27.663 | 68.790 | 1.00 41.30 |
| MOTA | 1774 | N | ASP | 239 | 20.174 | 27.776 | 69.194 | 1.00 37.96 |
| | 1775 | CA | ASP | 239 | 19.950 | 26.345 | 69.058 | 1.00 34.93 |
| MOTA | 1776 | CB | ASP | 239 | 19.748 | 25.735 | 70.449 | 1.00 38.61 |
| MOTA | 1777 | CG | ASP | 239 | 19.415 | 24.262 | 70.399 | 1.00 41.94 |
| ATOM | 1778 | OD1 | | 239 | 18.237 | 23.928 | 70.170 | 1.00 42.16 |
| MOTA | 1779 | OD2 | ASP | 239 | 20.341 | 23.438 | 70.582 | 1.00 45.62 |
| MOTA | 1780 | C | ASP | 239 | 18.743 | 26.059 | 68.162 | 1.00 31.17 |
| MOTA | 1781 | 0 | ASP | 239 | 17.661 | 26.608 | 68.370 | 1.00 28.67 |
| MOTA | 1782 | N | ILE | 240 | 18.926 | 25.198 | 67.164 | 1.00 25.89 |
| MOTA | 1783 | CA | ILE | 240 | 17.834 | 24.882 | 66.252 | 1.00 22.33 |
| ATOM | 1784 | CB | ILE | 240 | 18.295 | 23.912 | 65.132 | 1.00 21.20 |
| MOTA | 1785 | CG2 | ILE | 240 | 17.099 | 23.518 | 64.256 | 1.00 17.39 |
| MOTA | 1786 | CG1 | ILE | 240 | 19.356 | 24.592 | 64.265 | 1.00 21.01 |
| MOTA | 1787 | CD1 | ILE | 240 | 20.042 | 23.665 | 63.267 | 1.00 21.65 |
| ATOM | 1788 | С | ILE | 240 | 16.609 | 24.312 | 66.970 | 1.00 19.27 |
| MOTA | 1789 | 0 | ILE | 240 | 15.495 | 24.756 | 66.719 | 1.00 21.10 |
| MOTA | 1790 | N | ARG | 241 | 16.808 | 23.352 | 67.870 | 1.00 19.73 |
| ATOM | 1791 | CA | ARG | 241 | 15.687 | 22.761 | 68.592 | 1.00 19.91 |
| ATOM | 1792 | CB | ARG | 241 | 16.167 | 21.604 | 69.472 | 1.00 18.67 |
| ATOM | 1793 | CG | ARG | 241 | 16.544 | 20.366 | 68.659 | 1.00 19.80 |
| MOTA | 1794 | CD | ARG | 241 | 17.266 | 19.307 | 69.474 | 1.00 21.32 |
| MOTA | 1795 | NE | ARG | 241 | 17.484 | 18.087 | 68.692 | 1.00 22.98 |
| MOTA | 1796 | CZ | ARG | 241 | 18.334 | 17.979 | 67.675 | 1.00 24.19 |
| MOTA | 1797 | | ARG | 241 | 19.068 | 19.018 | 67.302 | 1.00 25.28 |
| ATOM | 1798 | | ARG | 241 | 18.444 | 16.830 | 67.018 | 1.00 24.38 |
| MOTA | 1799 | С | ARG | 241 | 14.964 | 23.806 | 69.427 | 1.00 20.32 |
| | | | | | | | | |

| ATOM | 1800 | 0 | ARG | 241 | 13.727 | 23.803 | 69.520 | 1.00 19.66 |
|--------------|--------------|-----------|------------|------------|------------------|------------------|------------------|--------------------------|
| ATOM | 1801 | N | ALA | 242 | 15.730 | 24.707 | 70.034 | 1.00 19.52 |
| ATOM | 1802 | CA | ALA | 242 | 15.133 | 25.771 | 70.832 | 1.00 19.63 |
| ATOM | 1803 | CB | ALA | 242 | 16.227 | 26.580 | 71.524 | 1.00 20.26 |
| ATOM | 1804 | C | ALA | 242 | 14.312 | 26.662 | 69.896 | 1.00 19.55 |
| ATOM | 1805 | o | ALA | 242 | 13.233 | 27.133 | 70.267 | 1.00 21.30 |
| | 1806 | N | ALA | 243 | 14.804 | 26.874 | 68.676 | 1.00 18.14 |
| ATOM | | | | 243 | 14.074 | 27.700 | 67.707 | 1.00 18.14 |
| ATOM | 1807 | CA | ALA | 243 | 14.928 | 27.700 | 66.457 | 1.00 19.34 |
| ATOM | 1808 | CB | ALA | | | 27.031 | 67.326 | 1.00 18.03 |
| ATOM | 1809 | C | ALA | 243 | 12.748 | | 67.180 | |
| ATOM | 1810 | 0 | ALA | 243 | 11.731 12.769 | 27.701 | | 1.00 20.19 |
| ATOM | 1811 | N | VAL | 244 | | 25.710 24.969 | 67.157 66.818 | 1.00 21.10 |
| ATOM | 1812 | CA | VAL | 244 | 11.554 | | | 1.00 19.17 |
| MOTA | 1813 | CB | VAL | 244 | 11.842 | 23.457 | 66.632 | 1.00 18.81 |
| ATOM | 1814 | | VAL | 244 | 10.536 | 22.668 | 66.538 | 1.00 18.20 |
| MOTA | 1815 | | VAL | 244 | 12.671 | 23.245 | 65.361 | 1.00 17.47 |
| MOTA | 1816 | C | VAL | 244 | 10.521 | 25.146 | 67.927 | 1.00 20.06 |
| MOTA | 1817 | 0 | VAL | 244 | 9.336 | 25.348 | 67.660 | 1.00 19.30 |
| MOTA | 1818 | N | ARG | 245 | 10.972 | 25.073 | 69.174 | 1.00 21.06 |
| ATOM | 1819 | CA | ARG | 245 | 10.063 | 25.227 | 70.297 | 1.00 21.32 |
| MOTA | 1820 | CB | ARG | 245 | 10.780 | 24.907 | 71.615 | 1.00 21.31 |
| MOTA | 1821 | CG | ARG | 245 | 11.128 | 23.427 | 71.766 | 1.00 22.58 |
| MOTA | 1822 | CD | ARG | 245 | 11.472 | 23.053 | 73.209 | 1.00 25.04 |
| ATOM | 1823 | NE | ARG | 245 | 12.697 | 23.674 | 73.698 | 1.00 26.83 |
| ATOM | 1824 | CZ | ARG | 245 | 13.930 | 23.291 | 73.375 | 1.00 29.75 |
| ATOM | 1825 | NH1 | | 245 | 14.126 | 22.274 | 72.547 | 1.00 30.29 |
| ATOM | 1826 | NH2 | | 245 | 14.980 | 23.921 | 73.896 | 1.00 29.20 |
| ATOM | 1827 | С | ARG | 245 | 9.435 | 26.619 | 70.352 | 1.00 21.20 |
| ATOM | 1828 | 0 | ARG. | 245 | 8.236 | 26.749 | 70.605 | 1.00 21.04 |
| ATOM | 1829 | N | GLN | 246 | 10.231 | 27.653 | 70.095 | 1.00 22.00 |
| MOTA | 1830 | CA | GLN | 246 | 9.730 | 29.024 | 70.122 | 1.00 23.64 1.00 26.15 |
| MOTA | 1831 | CB | GLN | 246 | 10.877 10.464 | 30.012 31.464 | 69.919 70.076 | 1.00 26.15 1.00 29.62 |
| MOTA | 1832 1833 | CG CD | GLN GLN | 246 246 | 11.652 | 32.399 | 70.076 | 1.00 29.02 |
| ATOM ATOM | 1834 | | GLN | 246 | 12.600 | 32.222 | 70.822 | 1.00 35.40 |
| ATOM | 1835 | NE2 | | 246 | 11.609 | 33.404 | 69.185 | 1.00 34.94 |
| ATOM | 1836 | C C | GLN | 246 | 8.683 | 29.220 | 69.036 | 1.00 34.34 |
| | 1837 | 0 | GLN | 246 | 7.664 | 29.880 | 69.245 | 1.00 23.85 |
| ATOM | 1838 | N | TYR | 247 | 8.942 | 28.651 | 67.864 | 1.00 21.90 |
| ATOM | 1839 | CA | TYR | 247 | 7.999 | 28.751 | 66.761 | 1.00 21.66 |
| ATOM | 1840 | CB | TYR | 247 | 8.571 | 28.037 | 65.528 | 1.00 19.75 |
| ATOM | 1841 | CG | TYR | 247 | 7.579 | 27.795 | 64.419 | 1.00 20.83 |
| ATOM | 1842 | CD1 | TYR | 247 | 6.815 | 28.837 | 63.899 | 1.00 19.45 |
| ATOM | 1843 | CE1 | | 247 | 5.892 | 28.612 | 62.885 | 1.00 21.16 |
| ATOM | 1844 | CD2 | TYR | 247 | 7.398 | 26.517 | 63.891 | 1.00 21.25 |
| ATOM | 1845 | CE2 | TYR | 247 | 6.480 | 26.281 | 62.876 | 1.00 21.03 |
| ATOM | 1846 | CZ | TYR | 247 | 5.729 | 27.327 | 62.378 | 1.00 20.70 |
| ATOM | 1847 | ОН | TYR | 247 | 4.802 | 27.085 | 61.388 | 1.00 20.47 |
| MOTA | 1848 | С | TYR | 247 | 6.673 | 28.125 | 67.199 | 1.00 21.28 |
| MOTA | 1849 | 0 | TYR | 247 | 5.609 | 28.723 | 67.026 | 1.00 21.42 |
| ATOM | 1850 | N | MET | 248 | 6.746 | 26.929 | 67.782 | 1.00 20.26 |
| ATOM | 1851 | CA | MET | 248 | 5.556 | 26.219 | 68.258 | 1.00 21.53 |
| ATOM | 1852 | CB | MET | 248 | 5.951 | 24.872 | 68.884 | 1.00 21.82 |
| MOTA | 1853 | CG | MET | 248 | 6.426 | 23.815 | 67.882 | 1.00 21.90 |
| ATOM | 1854 | SD | MET | 248 | 7.248 | 22.415 | 68.688 | 1.00 26.67 |
| ATOM | 1855 | CE | MET | 248 | 5.858 | 21.537 | 69.370 | 1.00 24.87 |
| MOTA | 1856 | С | MET | 248 | 4.786 | 27.040 | 69.293 | 1.00 22.86 |
| ATOM | 1857 | 0 | MET | 248 | 3.554 | 27.155 | 69.231 | 1.00 21.83 |
| MOTA | 1858 | N | ALA | 249 | 5.518 | 27.606 | 70.247 | 1.00 21.40 |
| MOTA | 1859 | CA | ALA | 249 | 4.898 | 28.405 | 71.299 | 1.00 21.90 |
| MOTA | 1860 | CB | ALA | 249 | 5.926 | 28.738 | 72.369 | 1.00 21.23 |
| ATOM | 1861 | C | ALA | 249 | 4.252 | 29.687 | 70.778 | 1.00 21.43 |
| ATOM | 1862 | 0 | ALA | 249 | 3.099 | 29.979 | 71.105 | 1.00 22.72 |
| MOTA | 1863 | N | GLU | 250 | 4.989 | 30,448 | 69.970 | 1.00 22.09 |
| MOTA | 1864 | CA | GLU | 250 | 4.469 | 31.707 | 69.433 | 1.00 23.27 |
| MOTA | 1865 | CB | GLU | 250 | 5.549 | 32.454 | 68.649 | 1.00 22.04 |
| MOTA | 1866 | CG | GLU | 250 | 6.815 | 32.693 | 69.442 | 1.00 24.15 |
| MOTA | 1867 | CD OF1 | GLU | 250 | 7.629 | 33.860 | 68.923 | 1.00 24.35 |
| MOTA | 1868 | OE1 | | 250 | 7.549 | 34.169 | 67.719 69.729 | 1.00 25.60 1.00 25.39 |
| ATOM | 1869 1870 | OE2 C | GLU | 250 250 | 8.362 3.231 | 34.464 31.538 | 68.558 | 1.00 25.39 |
| ATOM | 1871 | 0 | GLU | 250 | 2.406 | 32.454 | 68.449 | 1.00 25.21 |
| ATOM | 1872 | N | VAL | 250 | 3.093 | 30.376 | 67.930 | 1.00 24.11 |
| MOTA | 1873 | CA | VAL | 251 | 1.927 | 30.376 | 67.094 | 1.00 24.81 |
| ATOM | 1874 | CB | VAL | 251 | 2.114 | 28.886 | 66.198 | 1.00 23.31 |
| ATOM | 1875 | CG1 | | 251 | 0.827 | 28.605 | 65.431 | 1.00 22.66 |
| ATOM | 1876 | CG2 | | 251 | 3.260 | 29.108 | 65.234 | 1.00 23.33 |
| | | | | | | | | |

| ATOM | 1877 | С | VAL | 251 | 0.693 | 29.927 | 67.970 | 1.00 | 25.72 |
|--------------|--------------|----------|------------|-----|-----------|------------------|--------|------|-------|
| ATOM | 1878 | 0 | VAL | 251 | -0.355 | 30.524 | 67.731 | 1.00 | 26.34 |
| ATOM | 1879 | N | GLU | 252 | 0.825 | 29.085 | 68.990 | | 25.88 |
| ATOM | 1880 | CA | GLU | 252 | -0.291 | 28.804 | 69.885 | 1.00 | 28.97 |
| ATOM | 1881 | СВ | GLU | 252 | 0.066 | 27.667 | 70.842 | 1.00 | 31.63 |
| ATOM | 1882 | CG | GLU | 252 | -1.076 | 27.268 | 71.762 | | 35.49 |
| ATOM | 1883 | CD | GLU | 252 | -0.739 | 26.078 | 72.633 | | 38.81 |
| | | OE1 | | 252 | -1.557 | 25.730 | 73.513 | | 41.32 |
| ATOM | 1884 | | | | | | | | 40.57 |
| ATOM | 1885 | OE2 | GLU | 252 | 0.343 | 25.486 | 72.438 | | |
| ATOM | 1886 | C | GLU | 252 | -0.713 | 30.026 | 70.686 | | 29.30 |
| ATOM | 1887 | 0 | GLU | 252 | -1.872 | 30.142 | 71.082 | | 28.02 |
| ATOM | 1888 | N | SER | 253 | 0.233 | 30.930 | 70.922 | 1.00 | 30.46 |
| ATOM | 1889 | CA | SER | 253 | -0.038 | 32.148 | 71.681 | | 32.50 |
| ATOM | 1890 | CB | SER | 253 | 1.209 | 32.572 | 72.450 | | 32.17 |
| MOTA | 1891 | OG | SER | 253 | 1.459 | 31.671 | 73.519 | | 39.52 |
| MOTA | 1892 | С | SER | 253 | -0.497 | 33.302 | 70.794 | | 31.92 |
| MOTA | 1893 | 0 | SER | 253 | -1.051 | 34.288 | 71.283 | 1.00 | 32.17 |
| MOTA | 1894 | N | GLY | 254 | -0.264 | 33.178 | 69.492 | 1.00 | 30.27 |
| MOTA | 1895 | CA | GLY | 254 | -0.665 | 34.227 | 68.571 | 1.00 | 27.52 |
| ATOM | 1896 | С | GLY | 254 | 0.429 | 35.249 | 68.330 | 1.00 | 26.04 |
| ATOM | 1897 | 0 | GLY | 254 | 0.259 | 36.178 | 67.541 | 1.00 | 28.43 |
| ATOM | 1898 | N | VAL | 255 | 1.556 | 35.083 | 69.013 | 1.00 | 25.10 |
| ATOM | 1899 | CA | VAL | 255 | 2.678 | 35.998 | 68.861 | 1.00 | 24.43 |
| ATOM | 1900 | CB | VAL | 255 | 3.806 | 35.637 | 69.836 | | 24.55 |
| ATOM | 1901 | | VAL | 255 | 5.016 | 36.530 | 69.601 | | 25.47 |
| ATOM | 1902 | | VAL | 255 | 3.299 | 35.782 | 71.264 | 1.00 | 27.69 |
| ATOM | 1903 | C | VAL | 255 | 3.209 | 35.966 | 67.433 | | 23.67 |
| ATOM | 1904 | o | VAL - | 255 | 3.667 | .36.981 | 66.901 | | 21.95 |
| ATOM | 1905 | N | TYR | 256 | 3.155 | 34.786 | 66.821 | 1.00 | 24.22 |
| | 1905 | | | | 3.597 | 34.700 | 65.441 | | 22.81 |
| ATOM | | CA | TYR | 256 | | | | | |
| ATOM | 1907 | CB | TYR | 256 | 4.856 | 33.739 | 65.356 | | 22.52 |
| MOTA | 1908 | CG | TYR | 256 | 5.361 | 33.602 | 63.935 | | 22.38 |
| ATOM | 1909 | CD1 | | 256 | 6.061 | 34.644 | 63.320 | | 22.41 |
| MOTA | 1910 | CE1 | TYR | 256 | 6.436 | 34.574 | 61.975 | | 23.46 |
| ATOM | 1911 | CD2 | TYR | 256 | 5.053 | 32.473 | 63.171 | | 23.14 |
| MOTA | 1912 | CE2 | TYR · | 256 | 5.419 | 32.388 | 61.825 | 1.00 | 22.31 |
| MOTA | 1913 | CZ | TYR | 256 | 6.108 | 33.443 | 61.234 | 1.00 | 25.45 |
| MOTA | 1914 | OH | TYR | 256 | 6.448 | 33.378 | 59.894 | | 23.06 |
| MOTA | 1915 | C | TYR | 256 | 2.476 | 33.950 | 64.645 | 1.00 | 22.89 |
| ATOM | 1916 | 0 | TYR | 256 | 1.860 | 32.995 | 65.107 | 1.00 | 20.80 |
| ATOM | 1917 | N | PRO | 257 | 2.188 | 34.465 | 63.441 | 1.00 | 23.79 |
| MOTA | 1918 | CD | PRO . | 257 | 1.258 | 33.861 | 62.468 | 1.00 | 25.59 |
| MOTA | 1919 | CÁ | PRO | 257 | 2.886 | 35.611 | 62.854 | 1.00 | 25.56 |
| ATOM | 1920 | CB | PRO | 257 | 2.485 | 35.542 | 61.379 | 1.00 | 26.50 |
| ATOM | 1921 | CG | PRO | 257 | 1.128 | 34.947 | 61.427 | 1.00 | 26.66 |
| ATOM | 1922 | C | PRO | 257 | 2.489 | 36.934 | 63.513 | 1.00 | 26.91 |
| ATOM | 1923 | 0 | PRO | 257 | 1.382 | 37.074 | 64.027 | | 26.07 |
| ATOM | 1924 | N | GLY | 258 | 3.412 | 37.889 | 63.501 | | 28.06 |
| ATOM | 1925 | CA | GLY | 258 | 3.141 | 39.182 | 64.092 | | 31.45 |
| ATOM | 1926 | C | GLY | 258 | 2.550 | 40.108 | 63.052 | | 33.08 |
| ATOM | 1927 | 0 | GLY | 258 | 2.454 | 39.750 | 61.875 | | 31.82 |
| ATOM | 1928 | N | GLU | 259 | 2.153 | 41.301 | 63.476 | | 33.88 |
| ATOM | 1929 | CA | GLU | 259 | 1.571 | 42.259 | 62.554 | | 35.72 |
| ATOM | 1930 | CB | GLU | 259 | 1.118 | 43.513 | 63.304 | | 37.56 |
| | | | | 259 | 0.153 | 44.376 | 62.519 | | 40.03 |
| MOTA MOTA | 1931 1932 | CG CD | GLU GLU | 259 | -1.186 | 44.376 | 62.319 | | 42.11 |
| | | | | | | | 61.534 | | 45.27 |
| ATOM | 1933 | OE1 | | 259 | -2.009 | 44.237 42.620 | | | |
| MOTA | 1934 | OE2 | | 259 | -1.421 | | 62.886 | | 44.73 |
| ATOM | 1935 | C | GLU | 259 | 2.606 | 42.629 | 61.498 | | 36.27 |
| ATOM | 1936 | 0 | GLU | 259 | 2.258 | 43.046 | 60.391 | | 38.03 |
| ATOM | 1937 | N | GLU | 260 | 3.881 | 42.468 | 61.844 | | 36.02 |
| MOTA | 1938 | CA | GLU | 260 | 4.976 | 42.780 | 60.930 | | 36.42 |
| MOTA | 1939 | CB | GLU | 260 | 6.318 | 42.804 | 61.673 | | 39.45 |
| MOTA | 1940 | CG | GLU | 260 | 6.264 | 43.354 | 63.087 | | 43.52 |
| MOTA | 1941 | CD | GLU | 260 | 5.723 | 42.347 | 64.088 | | 46.00 |
| MOTA | 1942 | | GLU | 260 | 6.384 | 41.306 | 64.306 | | 47.00 |
| MOTA | 1943 | OE2 | GLU | 260 | 4.637 | 42.596 | 64.656 | | 46.44 |
| MOTA | 1944 | С | GLU | 260 | 5.057 | 41.724 | 59.836 | | 35.35 |
| MOTA | 1945 | 0 | GLU | 260 | 5.677 | 41.940 | 58.797 | 1.00 | 34.80 |
| MOTA | 1946 | N | HIS | 261 | 4.434 | 40.577 | 60.084 | 1.00 | 34.70 |
| MOTA | 1947 | CA | HIS | 261 | 4.448 | 39.471 | 59.132 | 1.00 | 34.15 |
| MOTA | 1948 | CB | HIS | 261 | 4.760 | 38.164 | 59.857 | | 32.10 |
| MOTA | 1949 | CG | HIS | 261 | 6.004 | 38.213 | 60.687 | | 31.51 |
| ATOM | 1950 | | HIS | 261 | 6.200 | 38.019 | 62.013 | | 29.70 |
| ATOM | 1951 | ND1 | | 261 | 7.249 | 38.460 | 60.149 | | 30.98 |
| ATOM | 1952 | CE1 | | 261 | | 38.411 | 61.106 | | 28.80 |
| ATOM | 1953 | | HIS | 261 | 7.548 | 38.145 | 62.246 | | 28.77 |
| | | | | | | | | | |

| ATOM | 1954 | С | HIS | 261 | 3.110 | 39.330 | 58.424 | 1.00 35.41 |
|--------------|------|---------------|-----|-------|--------|--------|--------|------------|
| ATOM | 1955 | 0 | HIS | 261 | 2.912 | 38.408 | 57.631 | 1.00 35.55 |
| ATOM | 1956 | N | SER | 262 | 2.195 | 40.248 | 58.716 | 1.00 35.97 |
| ATOM | 1957 | CA | SER | 262 | 0.864 | 40.226 | 58.133 | 1.00 36.99 |
| ATOM | 1958 | СВ | SER | 262 | -0.173 | 40.483 | 59.227 | 1.00 35.31 |
| | 1959 | OG | SER | 262 | -0.052 | 39.540 | 60.279 | 1.00 37.80 |
| MOTA | | | | | | | | |
| MOTA | 1960 | C | SER | 262 | 0.703 | 41.254 | 57.014 | 1.00 38.31 |
| MOTA | 1961 | 0 | SER | 262 | 1.483 | 42.203 | 56.909 | 1.00 37.66 |
| MOTA | 1962 | N | PHE | 263 | -0.312 | 41.050 | 56.178 | 1.00 40.01 |
| ATOM | 1963 | CA | PHE | 263 | -0.600 | 41.955 | 55.066 | 1.00 41.82 |
| | 1964 | CB | PHE | 263 | -0.434 | 41.243 | 53.718 | 1.00 42.58 |
| ATOM | 1965 | CG | PHE | 263 | 0.969 | 40.797 | 53.429 | 1.00 43.74 |
| ATOM | 1966 | | PHE | 263 | 1.306 | 39.447 | 53.467 | 1.00 43.83 |
| | 1967 | | PHE | 263 | 1.954 | 41.727 | 53.110 | 1.00 44.25 |
| ATOM | | | | | | 39.029 | | |
| ATOM | 1968 | CE1 | | 263 | 2.605 | | 53.190 | 1.00 44.88 |
| ATOM | 1969 | CE2 | PHE | 263 | 3.254 | 41.322 | 52.832 | 1.00 45.05 |
| ATOM | 1970 | \mathbf{cz} | PHE | 263 | 3.583 | 39.970 | 52.871 | 1.00 45.70 |
| MOTA | 1971 | C | PHE | 263 | -2.026 | 42.482 | 55.169 | 1.00 42.76 |
| ATOM | 1972 | 0 | PHE | 263 | -2.827 | 41.984 | 55.961 | 1.00 41.84 |
| MOTA | 1973 | N | HIS | 264 | -2.333 | 43.491 | 54.359 | 1.00 44.75 |
| ATOM | 1974 | CA | HIS | 264 | -3.661 | 44.102 | 54.336 | 1.00 47.39 |
| ATOM | 1975 | CB | HIS | 264 | -3.719 | 45.285 | 55.303 | 1.00 48.50 |
| MOTA | 1976 | CG | HIS | 264 | -3.536 | 44.897 | 56.735 | 1.00 49.55 |
| | 1977 | | HIS | 264 | -2.580 | 45.229 | 57.635 | 1.00 49.70 |
| MOTA | | | | | | | | |
| MOTA | 1978 | | HIS | 264 | -4.394 | 44.037 | 57.386 | 1.00 49.75 |
| MOTA | 1979 | | HIS | 264 | -3.973 | 43.854 | 58.625 | 1.00 50.24 |
| MOTA | 1980 | NE2 | HIS | 264 | -2.874 | 44.565 | 58.801 | 1.00 49.74 |
| ATOM | 1981 | C | HIS | 264 | -4.020 | 44.576 | 52.931 | 1.00 47.60 |
| MOTA | 1982 | 0 | HIS | 264 | -5.144 | 44.275 | 52.483 | 1.00 48.91 |
| ATOM | 1983 | .OXT | HIS | 264 | -3.178 | 45.249 | 52.302 | 1.00 48.36 |
| ATOM | 1984 | C1 | KPL | 265 | 5.087 | 27.716 | 51.358 | 1.00 41.50 |
| ATOM | 1985 | C2 | KPL | 265 | 4.190 | 26.479 | 51.578 | 1.00 40.60 |
| | | | | | | | 52.846 | |
| MOTA | 1986 | C3 | KPL | 265 | 4.654 | 25.755 | | 1.00 39.94 |
| MOTA | 1987 | C4 | KPL | 265 | 2.727 | 26.938 | 51.779 | 1.00 41.78 |
| MOTA | 1988 | 01 | KPL | 265 | 2.243 | 27.630 | 50.619 | 1.00 43.47 |
| ATOM | 1989 | C5 | KPL | 265 | 4.309 | 25.525 | 50.360 | 1.00 40.08 |
| MOTA | 1990 | 02 | KPL | 265 | 3.322 | 25.239 | 49.713 | 1.00 38.16 |
| ATOM | 1991 | C6 | KPL | 265 | 5.636 | 24.923 | 49.944 | 1.00 39.07 |
| ATOM | 1992 | 03 | KPL | 265 | 6.653 | 25.170 | 50.562 | 1.00 40.08 |
| ATOM | 1993 | 04 | KPL | 265 | 5.695 | 24.104 | 48.874 | 1.00 38.37 |
| ATOM | 1994 | СВ | MET | 301 | 16.154 | 43.498 | 31.231 | 1.00 80.41 |
| | | | | | 15.177 | 44.253 | 30.325 | 1.00 81.85 |
| MOTA | 1995 | CG | MET | 301 | | | | |
| MOTA | 1996 | SD | MET | 301 | 13.933 | 45.244 | 31.185 | 1.00 84.34 |
| ATOM | 1997 | CE | MET | 301 | 12.458 | 44.235 | 30.946 | 1.00 83.29 |
| ATOM | 1998 | С | MET | 301 | 14.844 | 42.880 | 33.290 | 1.00 78.13 |
| MOTA | 1999 | О | MET | 301 | 15.030 | 44.035 | 33.680 | 1.00 78.18 |
| ATOM | 2000 | N | MET | 301 | 14.641 | 41.532 | 31.184 | 1.00 78.62 |
| ATOM | 2001 | CA | MET | 301 | 15.549 | 42.343 | 32.045 | 1.00 78.92 |
| ATOM | 2002 | N | LYS | 302 | 14.042 | 42.021 | 33.914 | 1.00 76.63 |
| ATOM | 2003 | CA | LYS | 302 | 13.300 | 42.378 | 35.118 | 1.00 75.10 |
| АТОМ | 2004 | ·CB | LYS | 302 | 11.941 | 42.982 | 34.740 | 1.00 75.44 |
| | 2005 | CG | LYS | 302 | 11.997 | 44.455 | 34.355 | 1.00 75.76 |
| ATOM ATOM | 2005 | | | 302 | 12.271 | 45.330 | 35.571 | 1.00 75.70 |
| | | CD | LYS | | | | | |
| ATOM | 2007 | CE | LYS | 302 | 11.149 | 45.212 | 36.594 | 1.00 75.44 |
| MOTA | 2008 | NZ | LYS | 302 | 11.411 | 46.017 | 37.817 | 1.00 75.82 |
| ATOM | 2009 | С | LYS | 302 | 13.091 | 41.203 | 36.082 | 1.00 73.54 |
| MOTA | 2010 | 0 | LYS | 302 | 13.159 | 41.380 | 37.300 | 1.00 74.12 |
| ATOM | 2011 | N | PRO | 303 | 12.847 | 39.987 | 35.554 | 1.00 71.41 |
| ATOM ~ | 2012 | CD | PRO | 303 | 12.659 | 38.812 | 36.425 | 1.00 70.80 |
| ATOM | 2013 | CA | PRO | 303 | 12.743 | 39.596 | 34.143 | 1.00 69.04 |
| ATOM | 2014 | CB | PRO | 303 | 12.752 | 38.074 | 34.213 | 1.00 69.91 |
| ATOM | 2015 | CG | PRO | 303 | 12.025 | 37.812 | 35.486 | 1.00 70.53 |
| | | | | 303 | 11.499 | 40.136 | 33.444 | 1.00 66.77 |
| ATOM ATOM | 2016 | C | PRO | 303 | 10.485 | 40.130 | 34.083 | 1.00 66.86 |
| | 2017 | 0 | PRO | | | | | |
| MOTA | 2018 | N | THR | 304 | 11.588 | 40.276 | 32.127 | 1.00 64.02 |
| ATOM | 2019 | CA | THR | 304 | 10.474 | 40.781 | 31.337 | 1.00 61.28 |
| ATOM | 2020 | CB | THR | 304 | 10.830 | 40.818 | 29.842 | 1.00 61.21 |
| MOTA | 2021 | OG1 | THR | 304 | 12.085 | 41.486 | 29.668 | 1.00 60.91 |
| MOTA | 2022 | CG2 | THR | 304 | 9.756 | 41.560 | 29.062 | 1.00 60.88 |
| MOTA | 2023 | С | THR | 304 | 9.247 | 39.897 | 31.525 | 1.00 59.60 |
| MOTA | 2024 | ō | THR | 304 | 9.357 | 38.673 | 31.563 | 1.00 59.05 |
| ATOM | 2025 | N | THR | 305 | 8.079 | 40.522 | 31.644 | 1.00 57.62 |
| ATOM | 2026 | CA | THR | 305 | 6.836 | 39.783 | 31.829 | 1.00 55.83 |
| ATOM | 2027 | CB | THR | 305 | 6.207 | 40.074 | 33.204 | 1.00 55.66 |
| | | | | | 5.873 | 41.465 | 33.293 | 1.00 55.27 |
| ATOM | 2028 | OG1 | THR | 305 | | | | |
| ATOM | 2029 | CG2 | | . 305 | 7.176 | 39.713 | 34.317 | 1.00 55.55 |
| ATOM | 2030 | С | THR | 305 | 5.810 | 40.133 | 30.758 | 1.00 55.15 |
| | | | | | | | | |

| MOTA | 2031 | 0 | THR | 305 | 5.968 | 41.108 | 30.020 | 1.00 54.85 |
|--------|------|-----|-----|------------|----------------|------------------|--------|--------------------------|
| MOTA | 2032 | N | ILE | 306 | 4.756 | 39.328 | 30.680 | 1.00 54.30 |
| ATOM | 2033 | CA | ILE | 306 | 3.698 | 39.543 | 29.704 | 1.00 54.29 |
| ATOM | 2034 | СВ | ILE | 306 | 2.606 | 38.462 | 29.821 | 1.00 54.32 |
| ATOM | 2035 | CG2 | ILE | 306 | 1.645 | 38.567 | 28.644 | 1.00 54.60 |
| | | CG1 | ILE | 306 | 3.249 | 37.074 | 29.846 | 1.00 54.90 |
| MOTA | 2036 | | | | | | | |
| MOTA | 2037 | CD1 | ILE | 306 | 2.276 | 35.949 | 30.142 | 1.00 55.32 |
| MOTA | 2038 | C | ILE | 306 | 3.061 | 40.905 | 29.940 | 1.00 54.16 |
| MOTA | 2039 | 0 | ILE | 306 | 2.648 | 41.584 | 28.999 | 1.00 53.93 |
| MOTA | 2040 | N | SER | 307 | 2.990 | 41.299 | 31.208 | 1.00 53.96 |
| MOTA | 2041 | CA | SER | 307 | 2.402 | 42.579 | 31.588 | 1.00 54.22 |
| MOTA | 2042 | CB | SER | 307 | 2.523 | 42.777 | 33.101 | 1.00 54.20 |
| MOTA | 2043 | OG | SER | 307 | 1.851 | 41.744 | 33.801 | 1.00 55.29 |
| ATOM | 2044 | С | SER | 307 | 3.064 | 43.745 | 30.855 | 1.00 53.77 |
| ATOM | 2045 | Ō | SER | 307 | 2.383 | 44.653 | 30.379 | 1.00 54.19 |
| ATOM | 2046 | N | LEU | 308 | 4.392 | 43.712 | 30.770 | 1.00 53.02 |
| ATOM | 2047 | CA | LEU | 308 | 5.142 | 44.761 | 30.092 | 1.00 53.53 |
| | 2048 | CB | LEU | 308 | 6.630 | 44.411 | 30.049 | 1.00 53.40 |
| ATOM | | | | | | | | |
| ATOM | 2049 | CG | LEU | 308 | 7.434 | 44.783 | 31.295 | 1.00 54.50 |
| ATOM | 2050 | | LEU | 308 | 8.837 | 44.205 | 31.202 | 1.00 54.63 |
| MOTA | 2051 | | LEU | 308 | 7.487 | 46.304 | 31.424 | 1.00 54.20 |
| MOTA | 2052 | С | LEU | 308 | 4.631 | 44.988 | 28.676 | 1.00 53.65 |
| MOTA | 2053 | 0 | LEU | 308 | 4.355 | 46.120 | 28.277 | 1.00 53.25 |
| MOTA | 2054 | N | LEU | 309 | 4.509 | 43.905 | 27.917 | 1.00 53.27 |
| MOTA | 2055 | CA | LEU | 309 | 4.024 | 43.990 | 26.549 | 1.00 53.60 |
| ATOM | 2056 | CB | LEU | 309 | 3.994 | 42.599 | 25.914 | 1.00 53.39 |
| ATOM | 2057 | CG | LEU | 309 | 5.336 | 41.872 | 25.803 | 1.00 53.15 |
| ATOM | 2058 | | LEU | 309 | 5.108 | 40.469 | 25.271 | 1.00 52.80 |
| ATOM | 2059 | | LEU | 309 | 6.272 | 42.646 | 24.890 | 1.00 52.50 |
| | 2060 | | LEU | 309 | 2.625 | 44.598 | 26.530 | 1.00 53.99 |
| MOTA | | C | | | | | | |
| ATOM | 2061 | 0 | LEU | 309 | 2.312 | 45.429 | 25.677 | |
| ATOM | 2062 | N | GLN | 310 | 1.790 | 44.182 | 27.479 | 1.00 54.06 |
| ATOM | 2063 | CA | GLN | 310 | 0.425 | 44.685 | 27.576 | 1.00 55.21 |
| ATOM | 2064 | CB | GLN | 310 | -0.319 | 43.979 | 28.716 | 1.00 55.07 |
| MOTA | 2065 | CG | GLN | 310 | -1.810 | 44.283 | 28.790 | 1.00 55.61 |
| MOTA | 2066 | CD | GLN | 310 | -2.577 | 43.772 | 27.581 | 1.00 56.41 |
| MOTA | 2067 | OE1 | GLN | 310 | -2.395 | 44.254 | 26.463 | 1.00 56.40 |
| ATOM | 2068 | NE2 | GLN | 310 | -3.438 | 42.784 | 27.803 | 1.00 57.08 |
| ATOM | 2069 | С | GLN | 310 | 0.441 | 46.192 | 27.824 | 1.00 56.02 |
| ATOM | 2070 | ō | GLN | 310 | -0.263 | 46.949 | 27.153 | 1.00 56.00 |
| ATOM | 2071 | N | LYS | 311 | 1.252 | 46.620 | 28.786 | 1.00 56.45 |
| ATOM | 2072 | CA | LYS | 311 | 1.366 | 48.036 | 29.121 | 1.00 57.85 |
| | | | | | 2.361 | | 30.266 | 1.00 57.05 |
| MOTA | 2073 | CB | LYS | 311 | | 48.236 | | |
| ATOM | 2074 | CG | LYS | 311 | 2.419 | 49.668 | 30.777 | 1.00 59.71 |
| ATOM · | 2075 | CD | LYS | 311 | 3.851 | 50.156 | 30.939 | 1.00 60.00 |
| ATOM | 2076 | CE | LYS | 311 | 4.611 | 49.364 | 31.989 | 1.00 60.14 |
| MOTA | 2077 | NZ | LYS | 311 | 6.013 | 49.849 | 32.114 | 1.00 59.97 |
| ATOM | 2078 | С | LYS | 311 | 1.829 | 48.836 | 27.906 | 1.00 57.84 |
| ATOM | 2079 | 0 | LYS | 311 | 1.341 | 49.938 | 27.654 | 1.00 57.02 |
| ATOM | 2080 | N | TYR | 312 | 2.774 | 48.269 | 27.160 | 1.00 58.58 |
| ATOM | 2081 | CA | TYR | 312 | 3.316 | 48.913 | 25.970 | 1.00 59.79 |
| ATOM | 2082 | СВ | TYR | 312 | 4.369 | 48.014 | 25.314 | 1.00 60.90 |
| ATOM | 2083 | CG | TYR | 312 | 5.642 | 47.839 | 26.119 | 1.00 62.17 |
| ATOM | 2084 | CD1 | | 312 | 6.639 | 46.960 | 25.695 | 1.00 62.63 |
| ATOM | 2085 | CE1 | TYR | 312 | 7.818 | 46.799 | 26.424 | 1.00 63.39 |
| | | | | | | | 27.297 | |
| | 2086 | CD2 | TYR | 312 312 | 5.855 7.030 | 48.557 48.404 | 28.033 | 1.00 62.71 1.00 63.56 |
| MOTA | 2087 | CE2 | TYR | | | | | |
| ATOM | 2088 | CZ | TYR | 312 | 8.006 | 47.523 | 27.590 | 1.00 63.51 |
| ATOM | 2089 | ОН | TYR | 312 | 9.170 | 47.369 | 28.311 | 1.00 63.95 |
| ATOM | 2090 | C | TYR | 312 | 2.230 | 49.243 | 24.954 | 1.00 60.36 |
| ATOM | 2091 | 0 | TYR | 312 | 2.287 | 50.279 | 24.289 | 1.00 60.60 |
| ATOM | 2092 | N | LYS | 313 | 1.244 | 48.360 | 24.830 | 1.00 60.33 |
| MOTA | 2093 | CA | LYS | 313 | 0.155 | 48.579 | 23.887 | 1.00 60.59 |
| MOTA | 2094 | CB | LYS | 313 | -0.720 | 47.324 | 23.773 | 1.00 59.68 |
| ATOM | 2095 | CG | LYS | 313 | -1.855 | 47.466 | 22.766 | 1.00 59.36 |
| ATOM | 2096 | CD | LYS | 313 | -2.535 | 46.141 | 22.466 | 1.00 57.36 |
| ATOM | 2097 | CE | LYS | 313 | -3.587 | 46.318 | 21.377 | 1.00 57.43 |
| ATOM | 2098 | NZ | | 313 | -4.149 | 45.027 | 20.902 | 1.00 57.43 |
| | | | LYS | | -0.689 | 49.771 | 24.330 | 1.00 60.98 |
| ATOM | 2099 | С | LYS | 313 | | | | |
| ATOM | 2100 | 0 | LYS | 313 | -1.155 | 50.558 | 23.505 | 1.00 60.46 |
| MOTA | 2101 | N | GLN | 314 | -0.876 | 49.903 | 25.638 | 1.00 61.89 |
| ATOM | 2102 | CA | GLN | 314 | -1.656 | 51.004 | 26.186 | 1.00 63.46 |
| MOTA | 2103 | CB | GLN | 314 | -1.968 | 50.747 | 27.661 | 1.00 63.34 |
| ATOM | 2104 | CG | GLN | 314 | -2.812 | 49.507 | 27.898 | 1.00 64.06 |
| ATOM | 2105 | CD | GLN | 314 | -3.090 | 49.266 | 29.366 | 1.00 64.42 |
| ATOM | 2106 | OE1 | GLN | 314 | -3.675 | 50.108 | 30.047 | 1.00 64.71 |
| ATOM | 2107 | NE2 | | 314 | -2.672 | 48.110 | 29.862 | 1.00 64.63 |
| | | | | | | | | |

| ATOM | 2108 | С | GLN | 314 | -0.890 | 52.313 | 26.040 | 1.00 64.13 |
|--------------|--------------|-----------|------------|------------|------------------|------------------|------------------|--------------------------|
| MOTA | 2109 | 0 | GLN | 314 | -1.399 | 53.383 | 26.378 | 1.00 65.09 |
| ATOM · | 2110 | N | GLU | 315 | 0.336 | 52.217 | 25.533 | 1.00 64.44 |
| MOTA | 2111 | CA | GLU | 315 | 1.186 | 53.386 | 25.332 | 1.00 64.89 |
| MOTA | 2112 2113 | CB CG | GLU | 315 315 | 2.476 2.250 | 53.254 53.017 | 26.149 27.632 | 1.00 65.03 1.00 65.70 |
| ATOM ATOM | 2114 | CD | GLU | 315 | 3.548 | 52.910 | 28.407 | 1.00 65.70 |
| ATOM | 2115 | OE1 | | 315 | 4.414 | 52.101 | 28.013 | 1.00 66.19 |
| ATOM | 2116 | OE2 | | 315 | 3.702 | 53.631 | 29.414 | 1.00 66.44 |
| ATOM | 2117 | С | GLU | 315 | 1.532 | 53.541 | 23.855 | 1.00 64.71 |
| MOTA | 2118 | 0 | GLU | 315 | 2.323 | 54.408 | 23.480 | 1.00 64.82 |
| ATOM | 2119 | N | LYS | 316 | 0.938 | 52.692 | 23.023 | 1.00 64.19 |
| ATOM | 2120 2121 | CA | LYS | 316 316 | 1.176 0.604 | 52.731 54.024 | 21.585 20.997 | 1.00 64.21 1.00 64.07 |
| ATOM ATOM | 2121 | CB CG | LYS LYS | 316 | -0.840 | 54.024 | 21.387 | 1.00 64.07 |
| ATOM | 2123 | CD | LYS | 316 | -1.794 | 53.259 | 20.837 | 1.00 63.85 |
| ATOM | 2124 | CE | LYS | 316 | -3.220 | 53.514 | 21.306 | 1.00 63.79 |
| MOTA | 2125 | NZ | LYS | 316 | -3.703 | 54.874 | 20.934 | 1.00 63.74 |
| MOTA | 2126 | С | LYS | 316 | 2.671 | 52.643 | 21.276 | 1.00 64.35 |
| ATOM | 2127 | 0 | LYS | 316 | 3.157 | 53.260 | 20.327 | 1.00 64.34 |
| ATOM ATOM | 2128 2129 | N CA | LYS LYS | 317 317 | 3.395 4.835 | 51.876 51.702 | 22.087 21.907 | 1.00 64.27 1.00 63.70 |
| ATOM | 2130 | CB | LYS | 317 | 5.553 | 51.810 | 23.257 | 1.00 64.31 |
| АТОМ | 2131 | CG | LYS | 317 | 7.061 | 51.596 | 23.178 | 1.00 65.23 |
| | 2132 | CD | LYS | 317 | 7.689 | 51.451 | 24.560 | 1.00 65.71 |
| MOTA | 2133 | CE | LYS | 317 | 7.548 | 52.720 | 25.387 | 1.00 66.37 |
| ATOM | 2134. | NZ | LYS | 317 | 8.145 | 52.562 | 26.744 | 1.00 66.68 |
| ATOM | 2135 | C | LYS | 317 | 5.157 | 50.349 | 21.273 21.964 | 1.00 62.73 |
| ATOM ATOM | 2136 2137 | O N | LYS ARG | 317 318 | 5.221 5.361 | 49.331 50.342 | 19.959 | 1.00 62.19 1.00 61.20 |
| ATOM | 2138 | CA | ARG | 318 | 5.682 | 49.109 | 19.250 | 1.00 59.98 |
| ATOM | 2139 | CB | ARG | 318 | 5.760 | 49.370 | 17.743 | 1.00 60.40 |
| MOTA | 2140 | CG | ARG | 318 | 4.416 | 49.244 | 17.040 | 1.00 61.29 |
| MOTA | 2141 | CD | ARG | 318 | 4.469 | 49.737 | 15.604 | 1.00 61.24 |
| MOTA | 2142 | NE | ARG | 318 | 4.450 | 51.196 | 15.528 | 1.00 62.30 |
| ATOM | 2143 2144 | CZ NH1 | ARG | 318 318 | 4.415 4.397 | 51.885 51.249 | 14.392 13.227 | 1.00 62.88 1.00 62.95 |
| ATOM ATOM | 2144 | NH2 | ARG | 318 | 4.391 | 53.211 | 14.421 | 1.00 62.95 |
| ATOM | 2146 | С | ARG | 318 | 6.990 | 48.507 | 19.754 | 1.00 58.84 |
| MOTA | 2147 | 0 | ARG | 318 | 8.024 | 49.174 | 19.780 | 1.00 58.27 |
| MOTA | 2148 | N | PHE | 319 | 6.928 | 47.241 | 20.156 | 1.00 57.39 |
| MOTA | 2149 | CA | PHE | 319 | 8.089 | 46.530 | 20.677 | 1.00 55.69 |
| ATOM | 2150 | CB | PHE | 319 | 7.725 6.465 | 45.856 | 22.005 | 1.00 56.21 1.00 56.77 |
| ATOM ATOM | 2151 2152 | CG CD1 | PHE | 319 319 | 6.465 | 45.036 43.768 | 21.945 21.368 | 1.00 56.77 1.00 56.74 |
| ATOM | 2153 | CD2 | | 319 | 5.270 | 45.543 | 22.448 | 1.00 56.37 |
| ATOM | 2154 | CE1 | | 319 | 5.291 | 43.018 | 21.294 | 1.00 57.23 |
| MOTA | 2155 | CE2 | PHE | 319 | 4.092 | 44.803 | 22.379 | 1.00 56.83 |
| ATOM | 2156 | CZ | PHE | 319 | 4.101 | 43.539 | 21.801 | 1.00 56.54 |
| ATOM | 2157 | C | PHE | 319 | 8.632 | 45.497 | 19.692 | 1.00 54.04 |
| ATOM | 2158 2159 | O N | PHE ALA | 319 | 7.932 9.887 | 45.063 45.106 | 18.776 19.890 | 1.00 53.79 1.00 51.83 |
| MOTA MOTA | 2160 | N CA | ALA | 320 320 | 10.527 | 44.135 | 19.013 | 1.00 31.83 |
| ATOM | 2161 | CB | ALA | 320 | 11.880 | 44.665 | 18.562 | 1.00 49.67 |
| MOTA | 2162 | С | ALA | 320 | 10.695 | 42.773 | 19.676 | 1.00 47.51 |
| MOTA | 2163 | 0 | ALA | 320 | 10.899 | 42.677 | 20.886 | 1.00 47.41 |
| MOTA | 2164 | N | THR | 321 | 10.607 | 41.721 | 18.869 | 1.00 45.20 |
| MOTA | 2165 | CA | THR | 321 | 10.755 | 40.355 | 19.357 19.579 | 1.00 43.60 1.00 43.59 |
| MOTA MOTA | 2166 2167 | CB OG1 | THR | 321 321 | 9.383 8.618 | 40.472 | 20.506 | 1.00 43.39 |
| ATOM | 2168 | | THR | 321 | 9.553 | 38.293 | 20.132 | 1.00 44.04 |
| MOTA | 2169 | C | THR | 321 | 11.536 | 39.542 | 18.331 | 1.00 41.76 |
| MOTA | 2170 | 0 | THR | 321 | 11.456 | 39.804 | 17.130 | 1.00 41.89 |
| MOTA | 2171 | N | ILE | 322 | 12.290 | 38.551 | 18.798 | 1.00 40.55 |
| MOTA | 2172 | CA | ILE | 322 | 13.077 | 37.729 | 17.887 | 1.00 38.74 |
| ATOM | 2173 | CB CG2 | ILE ILE | 322 322 | 14.479 15.310 | 38.338 38.150 | 17.688 18.954 | 1.00 39.69 1.00 38.21 |
| MOTA MOTA | 2174 2175 | CG2 | ILE | 322 | 15.160 | 37.692 | 16.479 | 1.00 38.21 |
| ATOM | 2176 | | ILE | 322 | 16.436 | 38.388 | 16.055 | 1.00 40.64 |
| ATOM | 2177 | C | ILE | 322 | 13.220 | 36.289 | 18.375 | 1.00 37.51 |
| MOTA | 2178 | 0 | ILE | 322 | 13.037 | 36.005 | 19.557 | 1.00 36.20 |
| MOTA | 2179 | N | THR | 323 | 13.544 | 35.381 | 17.458 | 1.00 35.23 |
| MOTA | 2180 | CA | THR | 323 | 13.718 | 33.980 | 17.817 | 1.00 33.67 |
| ATOM ATOM | 2181 2182 | CB OG1 | THR THR | 323 323 | 13.381 14.346 | 33.034 33.202 | 16.640 15.596 | 1.00 33.56 1.00 33.89 |
| ATOM | 2182 | CG2 | THR | 323 | 11.996 | 33.331 | 16.096 | 1.00 33.03 |
| MOTA | 2184 | C | THR | 323 | 15.158 | 33.717 | 18.244 | 1.00 31.77 |

| MOTA | 2185 | 0 | THR | 323 | 16.071 | 34.459 | 17.879 | 1.00 30.93 |
|--------------|----------------------|--------|-----|------------|------------------|------------------|------------------|--------------------------|
| ATOM | 2186 | N | ALA | 324 | 15.345 | 32.661 | 19.033 | 1.00 30.73 |
| | | | ALA | 324 | 16.662 | 32.257 | 19.518 | 1.00 27.91 |
| MOTA | 2187 | CA | | | | | | |
| MOTA | 2188 | CB | ALA | 324 | 17.022 | 33.025 | 20.783 | 1.00 29.81 |
| ATOM | 2189 | С | ALA | 324 | 16.618 | 30.758 | 19.800 | 1.00 28.38 |
| ATOM | 2190 | 0 | ALA | 324 | 15.618 | 30.247 | 20.312 | 1.00 26.39 |
| MOTA | 2191 | N | TYR | 325 | 17.703 | 30.059 | 19.472 | 1.00 27.03 |
| ATOM | 2192 | CA | TYR | 325 | 17.759 | 28.616 | 19.663 | 1.00 27.26 |
| | 2193 | CB | TYR | 325 | 17.603 | 27.909 | 18.315 | 1.00 25.23 |
| ATOM | | | | | | | | |
| MOTA | 2194 | CG | TYR | 325 | 16.645 | 28.596 | 17.372 | 1.00 24.94 |
| MOTA | 2195 | CD1 | TYR | 325 | 17.109 | 29.501 | 16.417 | 1.00 23.93 |
| MOTA | 2196 | CE1 | TYR | 325 | 16.234 | 30.125 | 15.533 | 1.00 25.04 |
| MOTA | 2197 | CD2 | TYR | 325 | 15.275 | 28.336 | 17.427 | 1.00 23.23 |
| MOTA | 2198 | CE2 | TYR | 325 | 14.392 | 28.954 | 16.552 | 1.00 22.55 |
| ATOM | 2199 | CZ | TYR | 325 | 14.876 | 29.845 | 15.606 | 1.00 24.69 |
| ATOM | 2200 | ОН | TYR | 325 | 14.003 | 30.434 | 14.723 | 1.00 25.39 |
| | | | | | | | 20.333 | 1.00 27.49 |
| ATOM | 2201 | С | TYR | 325 | 19.038 | 28.131 | | |
| MOTA | 2202 | 0 | TYR | 325 | 19.287 | 26.931 | 20.400 | 1.00 28.39 |
| MOTA | 2203 | N | ASP | 326 | 19.854 | 29.052 | 20.827 | 1.00 27.48 |
| MOTA | 2204 | CA | ASP | 326 | 21.082 | 28.647 | 21.488 | 1.00 27.27 |
| ATOM | 2205 | CB | ASP | 326 | 22.182 | 28.392 | 20.453 | 1.00 26.92 |
| ATOM | 2206 | CG | ASP | 326 | 22.645 | 29.661 | 19.767 | 1.00 27.37 |
| ATOM | 2207 | | ASP | 326 | 23.394 | 30.439 | 20.397 | 1.00 28.68 |
| | | | ASP | | | | 18.603 | 1.00 28.94 |
| ATOM | 2208 | | | 326 | 22.253 | 29.881 | | |
| MOTA | 2209 | С | ASP | 326 | 21.541 | 29.677 | 22.510 | 1.00 28.59 |
| ATOM | 2210 | 0 | ASP | 326 | 20.991 | 30.773 | 22.593 | 1.00 30.01 |
| MOTA | 2211 | N | TYR | 327 | 22.547. | 29.302 | 23.289 | 1.00 28.76 |
| ATOM | 2212 | CA | TYR | 327 | 23.106 | 30.152 | 24.332 | 1.00 30.47 |
| ATOM | 2213 | CB | TYR | 327 | 24.203 | 29.385 | 25.073 | 1.00 31.91 |
| ATOM | 2214 | CG | TYR | 327 | 24.997 | 30.215 | 26.057 | 1.00 35.27 |
| | | | | | 24.465 | | | 1.00 35.27 |
| MOTA | 2215 | CD1 | TYR | 327 | | 30.562 | 27.300 | |
| ATOM | 2216 | CE1 | | 327 | 25.196 | 31.331 | 28.209 | 1.00 37.29 |
| MOTA | 2217 | CD2 | TYR | 327 | 26.281 | 30.658 | 25.744 | 1.00 35.38 |
| ATOM | 2218 | CE2 | TYR | 327 | 27.018 | 31.427 | 26.643 | 1.00 36.93 |
| ATOM | 2219 | CZ | TYR | 327 | 26.472 | 31.759 | 27.869 | 1.00 37.24 |
| ATOM | 2220 | ОН | TYR | 327 | 27.198 | 32.521 | 28.755 | 1.00 37.97 |
| ATOM | 2221 | C | TYR | 327 | 23.677 | 31.461 | 23.793 | 1.00 30.48 |
| | 2222 | | TYR | 327 | 23.216 | 32.543 | 24.148 | 1.00 29.09 |
| ATOM | | 0 | | | | | | |
| MOTA | 2223 | N | SER | 328 | 24.685 | 31.347 | 22.935 | 1.00 31.30 |
| ATOM | 2224 | CA | SER | 328 | 25.350 | 32.509 | 22.364 | 1.00 31.80 |
| ATOM | 2225 | CB | SER | 328 | 26.252 | 32.077 | 21.208 | 1.00 31.10 |
| ATOM | 2226 | OG | SER | 328 | 27.287 | 31.231 | 21.685 | 1.00 31.34 |
| ATOM | 2227 | С | SER | 328 | 24.411 | 33.620 | 21.905 | 1.00 33.46 |
| ATOM | 2228 | 0 | SER | 328 | 24.409 | 34.712 | 22.478 | 1.00 35.08 |
| ATOM | 2229 | N | PHE | 329 | 23.608 | 33.353 | 20.882 | 1.00 33.75 |
| | | | | | | | | |
| MOTA | 2230 | CA | PHE | 329 | 22.695 | 34.373 | 20.380 | |
| ATOM | 2231 | CB | PHE | 329 | 21.957 | 33.876 | 19.134 | 1.00 36.14 |
| ATOM | 2232 | CG | PHE | 329 | 22.794 | 33.915 | 17.884 | 1.00 37.89 |
| ATOM | 2233 | CD1 | PHE | 329 | 23.396 | 32.760 | 17.391 | 1.00 37.32 |
| MOTA | 2234 | CD2 | PHE | 329 | 22.995 | 35.117 | 17.207 | 1.00 37.37 |
| MOTA | 2235 | CE1 | PHE | 329 | 24.185 | 32.803 | 16.243 | 1.00 37.40 |
| ATOM | 2236 | CE2 | PHE | 329 | 23.781 | 35.169 | 16.061 | 1.00 37.67 |
| ATOM | 2237 | CZ | PHE | 329 | 24.378 | 34.011 | 15.576 | 1.00 38.05 |
| ATOM | 223 9 | C | PHE | 329 | 21.691 | 34.872 | 21.415 | 1.00 36.35 |
| | | | | | | | | |
| ATOM | 2239 | 0 | PHE | 329 | 21.294 | 36.040 | 21.387 | 1.00 35.47 |
| ATOM | 2240 | N | ALA | 330 | 21.282 | 33.997 | 22.328 | 1.00 36.19 |
| MOTA | 2241 | CA | ALA | 330 | 20.329 | 34.382 | 23.363 | 1.00 37.22 |
| MOTA | 2242 | CB | ALA | 330 | 19.929 | 33.159 | 24.187 | 1.00 37.12 |
| ATOM | 2243 | С | ALA | 330 | 20.930 | 35.453 | 24.275 | 1.00 38.43 |
| ATOM | 2244 | ō | ALA | 330 | 20.284 | 36.456 | 24.587 | 1.00 36.62 |
| ATOM | 2245 | N | LYS | 331 | 22.169 | 35.224 | 24.703 | 1.00 40.16 |
| MOTA | 2245 | CA | LYS | 331 | 22.877 | 36.150 | 25.583 | 1.00 42.64 |
| | | | | | | | | |
| MOTA | 2247 | CB | LYS | 331 | 24.239 | 35.560 | 25.970 | 1.00 43.34 |
| MOTA | 2248 | CG | LYS | 331 | 25.056 | 36.401 | 26.947 | 1.00 45.59 |
| MOTA | 2249 | CD | LYS | 331 | 24.494 | 36.320 | 28.362 | 1.00 48.66 |
| ATOM | 2250 | CE | LYS | 331 | 25.388 | 37.032 | 29.378 | 1.00 48.88 |
| ATOM | 2251 | NZ | LYS | 331 | 25.439 | 38.510 | 29.177 | 1.00 50.22 |
| ATOM | 2252 | C | LYS | 331 | 23.084 | 37.497 | 24.892 | 1.00 42.88 |
| ATOM | 2253 | ō | LYS | 331 | 23.000 | 38.554 | 25.520 | 1.00 44.09 |
| | | | | | 23.351 | 37.446 | 23.524 | 1.00 43.08 |
| ATOM | 2254 | N | LEU | 332 | | | | |
| ATOM | 2255 | CA | LEU | 332 | 23.588 | 38.645 | 22.807 | 1.00 42.72 |
| MOTA | 2256 | CB | LEU | 332 | 24.020 | 38.249 | 21.393 | 1.00 42.60 |
| MOTA | 2257 | CG | LEU | 332 | 24.502 | 39.350 | 20.447 | 1.00 42.52 |
| MOTA | 2258 | CD1 | LEU | 332 | 25.490 | 38.763 | 19.448 | 1.00 41.43 |
| MOTA | | | LEU | 332 | 23.315 | 39.981 | 19.740 | 1.00 42.66 |
| AIOM | 2259 | | | | | | | |
| | | | | 332 | 22.372 | 39.565 | 22.754 | 1.00 43.40 |
| ATOM ATOM | 2259 2260 2261 | C O | LEU | 332 332 | 22.372 22.488 | 39.565 40.770 | 22.754 22.980 | 1.00 43.40 1.00 42.27 |

| ATOM | 2262 | N | PHE | 333 | 21.204 | 39.004 | 22.463 | 1.00 42.78 |
|--------------|-------|------|------|-------------------|----------------------------|----------------------------|--------|--------------------------|
| ATOM | 2263 | CA | PHE | 333 | 19.997 | 39.814 | 22.387 | 1.00 43.66 |
| | | | | | | • | | |
| ATOM | 2264 | CB | PHE | 333 | 18.818 | 38.983 | 21.880 | 1.00 43.29 |
| ATOM | 2265 | CG | PHE | 333 | 19.080 | 38.289 | 20.580 | 1.00 43.11 |
| ATOM | 2266 | CD1 | PHE | 333 | 19.750 | 38.942 | 19.548 | 1.00 42.14 |
| ATOM | 2267 | CD2 | PHE | 333 | 18.640 | 36.986 | 20.379 | 1.00 42.92 |
| ATOM | 2268 | CE1 | PHE | 333 | 19.977 | 38.306 | 18.334 | 1.00 42.67 |
| | | CE2 | | 333 | 18.860 | 36.341 | 19.169 | 1.00 42.88 |
| ATOM | 2269 | | PHE | | | | | |
| ATOM | 2270 | cz | PHE | 333 | 19.531 | 37.001 | 18.141 | 1.00 42.87 |
| ATOM | 2271 | С | PHE | 333 | 19.651 | 40.393 | 23.747 | 1.00 44.42 |
| ATOM | 2272 | 0 | PHE | 333 | 19.189 | 41.530 | 23.851 | 1.00 43.85 |
| ATOM | 2273 | N | ALA | 334 | 19.881 | 39.600 | 24.789 | 1.00 45.14 |
| ATOM | 2274 | CA | ALA | 334 | 19.592 | 40.017 | 26.154 | 1.00 45.59 |
| | 2275 | | | | 19.912 | 38.884 | 27.121 | 1.00 45.78 |
| MOTA | | CB | ALA | 334 | | | | |
| ATOM | 2276 | C | ALA | 334 | 20.376 | 41.263 | 26.538 | 1.00 45.65 |
| MOTA | 2277 | 0 | ALA | 334 | 19.837 | 42.179 | 27.162 | 1.00 46.18 |
| MOTA | 2278 | N | ASP | 335 | 21.649 | 41.296 | 26.160 | 1.00 45.92 |
| ATOM | 2279 | CA | ASP | 335 | 22.509 | 42.429 | 26.482 | 1.00 45.71 |
| ATOM | 2280 | CB | ASP | 335 | 23.977 | 42.019 | 26.388 | 1.00 44.57 |
| ATOM | 2281 | CG | ASP | 335 | 24.277 | 40.767 | 27.177 | 1.00 43.56 |
| ATOM | 2282 | | ASP | 335 | 23.536 | 40.484 | 28.141 | 1.00 43.70 |
| | | | | 335 | 25.258 | 40.071 | 26.840 | 1.00 43.87 |
| ATOM | 2283 | OD2 | ASP | | | | | |
| MOTA | 2284 | С | ASP | 335 | 22.262 | 43.629 | 25.585 | 1.00 46.23 |
| ATOM | 2285 | 0 | ASP | 335 | 22.912 | 44.660 | 25.733 | 1.00 46.45 |
| ATOM | 2286 | N | GLU | 336 | 21.324 | 43.491 | 24.654 | 1.00 47.36 |
| ATOM | 2287 | CA | GLU | 336 | 20.999 | 44.580 | 23.741 | 1.00 49.00 |
| ATOM | 2288 | CB | GLU | 336 | 21.063 | 44.099 | 22.290 | 1.00 49.86 |
| ATOM | 2289 | CG | GLU | 336 | 22.459 | 43.725 | 21.828 | 1.00 51.33 |
| MOTA | 2290 | CD | GLU | 336 | 23.450 | 44.861 | 22.006 | 1.00 52.76 |
| | | | | | | | | |
| ATOM | 2291 | | GLU | 336 | 23.232 | 45.943 | 21.418 | 1.00 53.76 |
| ATOM | 2292 | OE2 | GLU | 336 | 24.443 | 44.672 | 22.741 | 1.00 53.33 |
| MOTA | 2293 | С | GLU | 336 | 19.620 | 45.156 | 24.026 | 1.00 49.27 |
| MOTA | 2294 | 0 | GLU | 336 | 19.171 | 46.076 | 23.341 | 1.00 49.79 |
| ATOM . | 2295 | N | GLY | 337 | 18.948 | 44.608 | 25.033 | 1.00 49.15 |
| MOTA | 2296 | CA | GLY | 337 | 17.627 | 45.094 | 25.386 | 1.00 49.61 |
| MOTA | 2297 | С | GLY | 337 | 16.497 | 44.169 | 24.981 | 1.00 50.11 |
| ATOM | 2298 | ō | GLY | 337 | 15.372 | 44.318 | 25.458 | 1.00 49.98 |
| | | | | | | | | |
| MOTA | 2299 | N | LEU | 338 | 16.788 | 43.219 | 24.095 | 1.00 50.32 |
| MOŢA | 2300 | CA | LEU | 338 | 15.779 | 42.267 | 23.637 | 1.00 50.74 |
| MOTA | 2301 | CB | LEU | 338 | 16.108 | 41.781 | 22.223 | 1.00 50.90 |
| ATOM . | 2302 | CG | LEU | 338 | 15.750 | 42.728 | 21.079 | 1.00 51.60 |
| MOTA | 2303 | CD1 | LEU | 338 | 16.237 | 42.143 | 19.763 | 1.00 52.47 |
| MOTA | 2304 | CD2 | LEU | 338 | 14.243 | 42.943 | 21.044 | 1.00 52.43 |
| ATOM | 2305 | C | LEU | 338 | 15.674 | 41.073 | 24.575 | 1.00 50.23 |
| | | | | | 16.430 | | 24.459 | 1.00 50.85 |
| MOTA | 2306 | 0 | LEU | 338 | | 40.109 | | |
| MOTA | 2307 | N | ASN | 339 | 14.729 | 41.146 | 25.506 | 1.00 49.73 |
| MOTA | 2308 | CA | ASN | 339 | 14.514 | 40.076 | 26.469 | 1.00 48.47 |
| MOTA | 2309 | CB · | ASN | 339 . | 14.536 | 40.647 | 27.889 | 1.00 50.75 |
| MOTA | 2310 | CG | ASN | 339 | 15.942 | 40.986 | 28.359 | 1.00, 52.34 |
| ATOM | 2311 | OD1 | ASN | 339 | 16.706 | 40.105 | 28.759 | 1.00 52.97 |
| ATOM | 2312 | | ASN | 339 | 16.293 | 42.267 | 28.301 | 1.00 52.70 |
| ATOM | .2313 | C | ASN | 339 | 13.194 | 39.355 | 26.204 | 1.00 46.90 |
| | | | | | 12.490 | | 27.129 | |
| ATOM | 2314 | 0 | ASN | 339 | | 38.961 | | 1.00 46.89 |
| MOTA | 2315 | N | VAL | 340 | 12.865 | 39.195 | 24.927 | 1.00 44.67 |
| MOTA | 2316 | CA | VAL | 340 | 11.645 | 38.509 | 24.518 | 1.00 43.58 |
| MOTA | 2317 | CB | VAL | 340 | 10.563 | 39.501 | 24.072 | 1.00 43.60 |
| MOTA | 2318 | CG1 | VAL | 340 | 9.272 | 38.758 | 23.779 | 1.00 43.89 |
| MOTA | 2319 | CG2 | VAL | 340 | 10.343 | 40.550 | 25.147 | 1.00 43.92 |
| ATOM | 2320 | С | VAL | 340 | 11.991 | 37.597 | 23.345 | 1.00 42.70 |
| ATOM | 2321 | 0 | VAL | 340 | 11.806 | 37.959 | 22.182 | 1.00 42.88 |
| ATOM | 2322 | N | MET | 341 | 12.496 | 36.410 | 23.667 | 1.00 41.15 |
| | | | | | | | | |
| ATOM | 2323 | CA | MET | 341 | 12.910 | 35.436 | 22.664 | 1.00 37.91 |
| MOTA | 2324 | CB | MET | 341 | 14.278 | 34.874 | 23.056 | 1.00 38.70 |
| MOTA | 2325 | CG | MET | 341 | 15.403 | 35.893 | 22.946 | 1.00 38.98 |
| MOTA | 2326 | SD | MET | 341 | 16.816 | 35.520 | 23.975 | 1.00 43.33 |
| ATOM | 2327 | CE | MET | 341 | 16.743 | 36.882 | 25.141 | 1.00 41.65 |
| ATOM | 2328 | С | MET | 341 | 11.910 | 34.299 | 22.461 | 1.00 36.58 |
| ATOM | 2329 | ō | MET | 341 | 11.208 | 33.895 | 23.389 | 1.00 34.24 |
| ATOM | 2330 | N | LEU | 342 | 11.858 | 33.784 | 21.236 | 1.00 33.02 |
| | | | | | | | | |
| ATOM | 2331 | CA | LEU | 342 | 10.949 | 32.697 | 20.904 | 1.00 31.78 |
| MOTA | 2332 | CB | LEU | 342 | 9.873 | 33.204 | 19.930 | 1.00 33.59 |
| MOTA | 2333 | CG | LEU | 342 | 8.868 | 32.254 | 19.260 | 1.00 35.82 |
| MOTA | 2334 | CD1 | LEU | 342 | 9.491 | 31.606 | 18.041 | 1.00 36.45 |
| MOTA | 2225 | CD2 | LEU | 342 | 8.380 | 31.210 | 20.256 | 1.00 35.85 |
| | 2335 | | | | | | | |
| ATOM | 2336 | C | LEU. | 342 | 11.671 | 31.485 | 20.317 | 1.00 28.89 |
| ATOM ATOM | 2336 | | LEU. | | | | | 1.00 28.89 1.00 28.45 |
| | | С | | 342 342 343 | 11.671 12.390 11.494 | 31.485 31.594 30.334 | | |

| MOTA | 2339 | CA | VAL | 343 | 12.099 | 29.093 | 20.483 | 1.00 24.23 |
|--------|--------------|-----|-----|------------|------------------|------------------|---------|------------|
| ATOM | 2340 | СВ | VAL | 343 | 12.543 | 28.193 | 21.664 | 1.00 24.85 |
| ATOM | 2341 | | VAL | 343 | 13.222 | 26.942 | 21.135 | 1.00 24.17 |
| ATOM | 2342 | CG2 | | 343 | 13.490 | 28.960 | 22.585 | 1.00 24.85 |
| ATOM | 2343 | C | VAL | 343 | 11.001 | 28.393 | 19.685 | 1.00 23.87 |
| ATOM | 2344 | ō | VAL | 343 | 10.253 | 27.575 | 20.220 | 1.00 23.67 |
| ATOM | 2345 | N | GLY | 344 | 10.900 | 28.737 | 18.404 | 1.00 23.68 |
| ATOM | 2346 | CA | GLY | 344 | 9.871 | 28.152 | 17.562 | 1.00 24.64 |
| ATOM | 2347 | С | GLY | 344 | 10.312 | 26.961 | 16.736 | 1.00 23.93 |
| ATOM | 2348 | ō | GLY | 344 | 11.507 | 26.689 | 16.621 | 1.00 22.71 |
| ATOM | 2349 | N | ASP | 345 | 9.340 | 26.253 | 16.161 | 1.00 23.97 |
| ATOM | 2350 | CA | ASP | 345 | 9.625 | 25.087 | 15.342 | 1.00 24.30 |
| ATOM | 2351 | СВ | ASP | 345 | 8.342 | 24.306 | 15.022 | 1.00 26.36 |
| ATOM | 2352 | CG | ASP | 345 | 7.201 | 25.196 | 14.563 | 1.00 26.89 |
| ATOM | 2353 | | ASP | 345 | 7.454 | 26.315 | 14.068 | 1.00 27.29 |
| ATOM | 2354 | OD2 | | 345 | 6.042 | 24.759 | 14.691 | 1.00 28.98 |
| ATOM | 2355 | С | ASP | 345 | 10.337 | 25.464 | 14.051 | 1.00 25.12 |
| ATOM | 2356 | 0 | ASP | 345 | 10.707 | 24.597 | 13.260 | 1.00 25.35 |
| ATOM | 2357 | N | SER | 346 | 10.538 | 26.761 | 13.840 | 1.00 24.45 |
| ATOM | 2358 | CA | SER | 346 | 11.237 | 27.218 | 12.649 | 1.00 23.43 |
| ATOM | 2359 | СВ | SER | 346 | 11.273 | 28.749 | 12.603 | 1.00 23.92 |
| ATOM | 2360 | OG | SER | 346 | 11.844 | 29.276 | 13.786 | 1.00 27.17 |
| ATOM | 2361 | С | SER | 346 | 12.655 | 26.655 | 12.705 | 1.00 23.97 |
| ATOM | 2362 | O | SER | 346 | 13.330 | 26.533 | 11.685 | 1.00 24.80 |
| ATOM | 2363 | N | LEU | 347 | 13.090 | 26.295 | 13.909 | 1.00 22.27 |
| ATOM | 2364 | CA | LEU | 347 | 14.417 | 25.730 | 14.106 | 1.00 22.38 |
| ATOM | 2365 | СВ | LEU | 347 | 14.664 | 25.473 | 15.601 | 1.00 22.34 |
| ATOM | 2366 | CG | LEU | 347 | 13.793 | 24.461 | .16.355 | 1.00 23.80 |
| ATOM . | 2367 | CD1 | | 347 | 14.374 | 23.052 | 16.197 | 1.00 21.37 |
| ATOM | 2368 | | LEU | 347 | 13.746 | 24.838 | 17.831 | 1.00 22.86 |
| ATOM | 2369 | C | LEU | 347 | 14.548 | 24.426 | 13.313 | 1.00 21.48 |
| ATOM | 2370 | 0 | LEU | 347 | 15.653 | 23.970 | 13.033 | 1.00 22.19 |
| ATOM | 2371 | N | GLY | 348 | 13.413 | 23.835 | 12.955 | 1.00 22.76 |
| ATOM | 2372 | CA | GLY | 348 | 13.439 | 22.601 | 12.196 | 1.00 23.34 |
| ATOM | 2372 | C | GLY | 348 | 14.005 | 22.837 | 10.814 | 1.00 23.54 |
| ATOM | 2374 | 0 | GLY | 348 | 14.534 | 21.927 | 10.014 | 1.00 24.89 |
| | | | | | | | 10.175 | 1.00 25.57 |
| MOTA | 2375 2376 | N | MET | 349 349 | 13.908 14.408 | 24.078 24.431 | 9.034 | 1.00 25.37 |
| MOTA | | CA | MET | | | | | |
| ATOM | 2377 | CB | MET | 349 | 13.349 | 25.255 | 8.290 | 1.00 28.73 |
| ATOM | 2378 | CG | MET | 349 | 12.062 | 24.479 | 8.029 | 1.00 32.37 |
| MOTA | 2379 | SD | MET | 349 | 10.740 | 25.431 | 7.229 | 1.00 34.95 |
| ATOM | 2380 | CE | MET | 349 | 11.415 | 25.598 | 5.580 | 1.00 34.51 |
| ATOM | 2381 | C | MET | 349 | 15.729 | 25.191 | 9.118 | 1.00 27.11 |
| ATOM | 2382 | 0 | MET | 349 | 16.700 | 24.839 | 8.448 | 1.00 26.59 |
| ATOM | 2383 | N | THR | 350 | 15.774 | 26.205 | 9.975 | 1.00 27.84 |
| ATOM | 2384 | CA | THR | 350 | 16.965 | 27.031 | 10.133 | 1.00 28.17 |
| ATOM | 2385 | CB | THR | 350 | 16.594 | 28.375 | 10.805 | 1.00 31.28 |
| ATOM | 2386 | OG1 | THR | 350 | 17.720 | 29.258 | 10.770 | 1.00 34.87 |
| ATOM | 2387 | CG2 | THR | 350 | 16.181 | 28.151 | 12.249 | 1.00 31.41 |
| ATOM | 2388 | С | THR | 350 | 18.098 | 26.370 | 10.926 | 1.00 28.30 |
| ATOM | 2389 | 0 | THR | 350 | 19.275 | 26.666 | 10.713 | 1.00 27.38 |
| ATOM | 2390 | N | VAL | 351 | 17.747 | 25.470 | 11.836 | 1.00 26.54 |
| ATOM | 2391 | CA | VAL | 351 | 18.750 | 24.792 | 12.648 | 1.00 26.15 |
| ATOM | 2392 | CB | VAL | 351 | 18.337 | 24.800 | 14.136 | 1.00 27.12 |
| ATOM | 2393 | | VAL | 351 | 19.340 | 24.010 | 14.966 | 1.00 26.33 |
| MOTA | 2394 | CG2 | | 351 | 18.238 | 26.239 | 14.633 | 1.00 26.84 |
| ATOM | 2395 | C | VAL | 351 | 18.995 | 23.347 | 12.214 | 1.00 25.31 |
| ATOM | 2396 | 0 | VAL | 351 | 20.138 | 22.943 | 12.023 | 1.00 23.95 |
| MOTA | 2397 | N | GLN | 352 | 17.920 | 22.574 | 12.064 | 1.00 24.36 |
| ATOM . | 2398 | CA | GLN | 352 | 18.036 | 21.169 | 11.673 | 1.00 23.55 |
| MOTA | 23.99 | CB | GLN | 352 | 16.839 | 20.370 | 12.200 | 1.00 23.18 |
| MOTA | 2400 | CG | GLN | 352 | 16.508 | 20.642 | 13.670 | 1.00 21.36 |
| MOTA | 2401 | CD | GLN | 352 | 15.365 | 19.785 | 14.186 | 1.00 20.35 |
| MOTA | 2402 | | GLN | 352 | 14.468 | 19.417 | 13.434 | 1.00 19.01 |
| ATOM | 2403 | | GLN | 352 | 15.387 | 19.476 | 15.484 | 1.00 18.25 |
| MOTA | 2404 | C | GLN | 352 | 18.156 | 20.972 | 10.159 | 1.00 24.30 |
| ATOM | 2405 | 0 | GLN | 352 | 18.727 | 19.982 | 9.703 | 1.00 24.86 |
| ATOM | 2406 | N | GLY | 353 | 17.602 | 21.900 | 9.385 | 1.00 24.94 |
| MOTA | 2407 | CA | GLY | 353 | 17.688 | 21.796 | 7.938 | 1.00 26.08 |
| MOTA | 2408 | С | GLY | 353 | 16.607 | 20.985 | 7.245 | 1.00 28.43 |
| MOTA | 2409 | 0 | GLY | 353 | 16.866 | 20.335 | 6.229 | 1.00 29.40 |
| MOTA | 2410 | N | HIS | 354 | 15.393 | 21.020 | 7.781 | 1.00 28.07 |
| ATOM | 2411 | CA | HIS | 354 | 14.280 | 20.291 | 7.192 | 1.00 29.87 |
| MOTA | 2412 | CB | HIS | 354 | 13.328 | 19.807 | 8.286 | 1.00 28.92 |
| ATOM | 2413 | CG | HIS | 354 | 13.906 | 18.740 | 9.161 | 1.00 28.40 |
| MOTA | 2414 | | HIS | | 14.175 | 18.722 | 10.488 | 1.00 28.09 |
| ATOM | 2415 | ND1 | HIS | 354 | 14.272 | 17.501 | 8.679 | 1.00 28.16 |
| | | | | | | | | |

| ATOM | 2416 | CE1 | HIS | 354 | 14.741 | 16.766 | 9.671 | 1.00 28.40 |
|-------|------|-----|-----|------------|--------|--------|--------|------------|
| ATOM | 2417 | NE2 | HIS | 354 | 14.693 | 17.484 | 10.780 | 1.00 27.51 |
| ATOM | 2418 | C | HIS | 354 | 13.520 | 21.162 | 6.198 | 1.00 31.29 |
| ATOM | 2419 | 0 | HIS | 354 | 13.625 | 22.389 | 6.227 | 1.00 31.35 |
| ATOM | 2420 | N | ASP | 355 | 12.755 | 20.518 | 5.320 | 1.00 33.89 |
| • | 2421 | CA | ASP | 355 | 11.972 | 21.224 | 4.305 | 1.00 33.03 |
| MOTA | | | | | | | | |
| MOTA | 2422 | CB | ASP | 355 | 11.479 | 20.231 | 3.245 | 1.00 38.73 |
| MOTA | 2423 | CG | ASP | 355 | 10.673 | 19.085 | 3.842 | 1.00 41.27 |
| MOTA | 2424 | | ASP | 355 | 9.606 | 19.349 | 4.430 | 1.00 43.21 |
| MOTA | 2425 | OD2 | ASP | 355 | 11.109 | 17.916 | 3.719 | 1.00 44.12 |
| MOTA | 2426 | С | ASP | 355 | 10.786 | 21.953 | 4.928 | 1.00 34.04 |
| MOTA | 2427 | 0 | ASP | 355 | 10.248 | 22.898 | 4.348 | 1.00 33.77 |
| ATOM | 2428 | N | SER | 356 | 10.382 | 21.503 | 6.111 | 1.00 31.25 |
| MOTA | 2429 | CA | SER | 356 | 9.268 | 22.106 | 6.832 | 1.00 29.42 |
| MOTA | 2430 | CB | SER | 356 | 7.963 | 21.353 | 6.531 | 1.00 29.55 |
| ATOM | 2431 | OG | SER | 356 | 7.976 | 20.046 | 7.086 | 1.00 30.40 |
| ATOM | 2432 | c | SER | 356 | 9.564 | 22.058 | 8.330 | 1.00 26.94 |
| ATOM | 2433 | Õ | SER | 356 | 10.642 | 21.627 | 8.739 | 1.00 26.83 |
| | 2434 | N | THR | 357 | 8.612 | 22.498 | 9.145 | 1.00 26.28 |
| MOTA | | | | | | | | 1.00 24.80 |
| ATOM | 2435 | CA | THR | 357 | 8.803 | 22.491 | 10.592 | |
| ATOM | 2436 | CB | THR | 357 | 8.205 | 23.749 | 11.254 | 1.00 23.50 |
| ATOM | 2437 | OG1 | | 357 | 6.780 | 23.735 | 11.093 | 1.00 25.56 |
| ATOM | 2438 | CG2 | THR | 357 | 8.777 | 25.017 | 10.630 | 1.00 26.01 |
| MOTA | 2439 | С | THR | 357 | 8.141 | 21.288 | 11.252 | 1.00 22.76 |
| MOTA | 2440 | 0 | THR | 357 | 8.262 | 21.106 | 12.458 | 1.00 21.76 |
| MOTA | 2441 | N | LEU | 358 | 7.449 | 20.466 | 10.470 | 1.00 21.94 |
| MOTA | 2442 | CA | LEU | 358 | 6.757 | 19.306 | 11.036 | 1.00 20.73 |
| ATOM | 2443 | CB | LEU | 358 | 5.987 | 18.553 | 9.946 | 1.00 22.06 |
| ATOM | 2444 | CG | LEU | 358 | 4.696 | 19.207 | 9.447 | 1.00 22.23 |
| ATOM | 2445 | | LEU | 358 | 5.036 | 20.431 | 8.609 | 1.00 24.54 |
| MOTA | 2446 | | LEU | 358 | 3.901 | 18.213 | 8.623 | 1.00 21.61 |
| ATOM | 2447 | C | LEU | 358 | 7.620 | 18.311 | 11.807 | 1.00 19.69 |
| | | | | | 7.169 | | | 1.00 19.09 |
| ATOM | 2448 | 0 | LEU | 358 | | 17.732 | 12.792 | |
| | 2449 | N | PRO | 359 | 8.861 | 18.077 | 11.359 | 1.00 19.49 |
| MOTA | 2450 | CD | PRO | 359 | 9.445 | 18.471 | 10.067 | 1.00 20.99 |
| MOTA | 2451 | CA | PRO | 359 | 9.738 | 17.130 | 12.057 | 1.00 19.78 |
| MOTA | 2452 | CB | PRO | 359 | 10.917 | 16.974 | 11.095 | 1.00 21.23 |
| MOTA | 2453 | CG | PRO | 359 | 10.905 | 18.271 | 10.325 | 1.00 25.57 |
| MOTA | 2454 | С | PRO | 359 | 10.184 | 17.534 | 13.461 | 1.00 18.27 |
| ATOM. | 2455 | 0 | PRO | 359 | 10.685 | 16.705 | 14.225 | 1.00 16.56 |
| ATOM | 2456 | N | VAL | 360 | 9.993 | 18.800 | 13.806 | 1.00 17.80 |
| ATOM | 2457 | CA | VAL | 360 | 10.397 | 19.290 | 15.116 | 1.00 17.74 |
| ATOM | 2458 | | VAL | 360 | 10.204 | 20.816 | 15.226 | 1.00 16.25 |
| ATOM | 2459 | | VAL | 360 | 10.676 | 21.301 | 16.582 | 1.00 15.89 |
| ATOM | 2460 | CG2 | | 360 | 10.967 | 21.508 | 14.114 | 1.00 16.99 |
| ATOM | 2461 | C | VAL | 360 | 9.589 | 18.608 | 16.205 | 1.00 17.81 |
| | | | | | | 18.577 | | |
| MOTA | 2462 | 0 | VAL | 360 | 8.362 | | 16.152 | |
| ATOM | 2463 | N | THR | 361 | 10.280 | 18.056 | 17.195 | 1.00 18.83 |
| ATOM | 2464 | | THR | 361 | 9.594 | 17.376 | 18.283 | 1.00 19.94 |
| ATOM | 2465 | CB | THR | 361 | 10.216 | 15.983 | 18.540 | 1.00 23.20 |
| ATOM | 2466 | OG1 | | 361 | 10.537 | 15.352 | 17.289 | 1.00 26.54 |
| MOTA | 2467 | CG2 | THR | 361 | 9.221 | 15.091 | 19.257 | 1.00 27.25 |
| ATOM | 2468 | С | THR | 361 | 9.656 | 18.195 | 19.571 | 1.00 19.28 |
| ATOM | 2469 | Ο. | THR | 361 | 10.442 | 19.138 | 19.679 | 1.00 17.95 |
| ATOM | 2470 | N | VAL | 362 | 8.820 | 17.841 | 20.544 | 1.00 17.01 |
| ATOM | 2471 | CA | VAL | 362 | 8.807 | 18.545 | 21.827 | 1.00 17.54 |
| ATOM | 2472 | СВ | VAL | 362 | 7.753 | 17.930 | 22.787 | 1.00 16.12 |
| ATOM | 2473 | | VAL | 362 | 7.835 | 18.598 | 24.156 | 1.00 15.29 |
| ATOM | 2474 | | VAL | 362 | 6.352 | 18.108 | 22.198 | 1.00 16.25 |
| ATOM | 2475 | C | VAL | 362 | 10.202 | 18.463 | 22.450 | 1.00 16.96 |
| ATOM | 2476 | Õ | VAL | 362 | 10.703 | 19.445 | 22.989 | 1.00 16.86 |
| | | | | | 10.829 | 17.293 | 22.351 | |
| ATOM | 2477 | N | ALA | 363 | | | | |
| ATOM | 2478 | CA | ALA | 363 | 12.164 | 17.088 | 22.903 | 1.00 18.14 |
| MOTA | 2479 | СВ | ALA | 363 | 12.638 | 15.659 | 22.632 | 1.00 20.14 |
| ATOM | 2480 | С | ALA | 363 | 13.161 | 18.086 | 22.327 | 1.00 18.21 |
| MOŢA | 2481 | 0 | ALA | 363 | 14.042 | 18.574 | 23.043 | 1.00 17.54 |
| ATOM | 2482 | N | ASP | 364 | 13.029 | 18.378 | 21.032 | 1.00 16.91 |
| ATOM | 2483 | CA | ASP | 364 | 13.923 | 19.334 | 20.371 | 1.00 16.57 |
| ATOM | 2484 | CB | ASP | 364 | 13.661 | 19.410 | 18.854 | 1.00 15.99 |
| ATOM | 2485 | CG | ASP | 364 | 13.951 | 18.099 | 18.123 | 1.00 17.52 |
| ATOM | 2486 | | ASP | 364 | 14.817 | 17.312 | 18.572 | 1.00 15.98 |
| ATOM | 2487 | | ASP | 364 | 13.311 | 17.873 | 17.072 | 1.00 19.08 |
| ATOM | 2488 | C | ASP | | 13.691 | 20.720 | 20.974 | 1.00 15.38 |
| ATOM | 2489 | 0 | ASP | 364 | 14.638 | 21.421 | 21.320 | 1.00 17.32 |
| ATOM | | | | | 12.427 | 21.115 | 21.088 | 1.00 17.32 |
| | 2490 | N | ILE | 365 365 | | | | |
| ATOM | 2491 | CA | ILE | 365 | 12.092 | 22.422 | 21.651 | 1.00 16.80 |
| MOTA | 2492 | CB | ILE | 365 | 10.561 | 22.646 | 21.717 | 1.00 16.19 |

| ATOM | 2493 | CG2 | ILE | 365 | 10.265 | 23.986 | 22.395 | 1.00 19.39 |
|------|--------------|-----|------|-----|--------|------------------|--------|------------|
| ATOM | 2494 | CG1 | ILE | 365 | 9.946 | 22.599 | 20.310 | 1.00 16.26 |
| ATOM | 2495 | CD1 | ILE | 365 | 10.399 | 23.713 | 19.379 | 1.00 17.28 |
| ATOM | 2496 | C | ILE | 365 | 12.646 | 22.560 | 23.066 | 1.00 16.75 |
| ATOM | 2497 | Ö | ILE | 365 | 13.217 | 23.596 | 23.423 | 1.00 15.83 |
| | | | | 366 | 12.474 | | 23.423 | 1.00 15.83 |
| ATOM | 2498 | N | ALA | | | 21.518 | 25.260 | |
| ATOM | 2499 | CA | ALA | 366 | 12.959 | 21.549 | | 1.00 15.66 |
| ATOM | 2500 | CB | ALA | 366 | 12.533 | 20.278 | 25.999 | 1.00 15.05 |
| ATOM | 2501 | С | ALA | 366 | 14.474 | 21.688 | 25.292 | 1.00 15.90 |
| MOTA | 2502 | 0 | ALA | 366 | 15.036 | 22.363 | 26.161 | 1.00 16.01 |
| MOTA | 2503 | N | TYR | 367 | 15.136 | 21.040 | 24.341 | 1.00 15.21 |
| ATOM | 2504 | CA | TYR | 367 | 16.596 | 21.093 | 24.247 | 1.00 15.10 |
| MOTA | 2505 | CB | TYR | 367 | 17.082 | 20.191 | 23.106 | 1.00 14.11 |
| MOTA | 2506 | CG | TYR | 367 | 18.577 | 20.270 | 22.837 | 1.00 15.47 |
| MOTA | 2507 | CD1 | TYR | 367 | 19.504 | 19.782 | 23.755 | 1.00 15.21 |
| ATOM | 2508 | CE1 | TYR | 367 | 20.881 | 19.830 | 23.492 | 1.00 16.91 |
| MOTA | 2509 | CD2 | TYR | 367 | 19.060 | 20.815 | 21.651 | 1.00 17.33 |
| ATOM | 2510 | | TYR | 367 | 20.428 | 20.868 | 21.382 | 1.00 17.98 |
| ATOM | 2511 | CZ | TYR | 367 | 21.330 | 20.371 | 22.306 | 1.00 16.29 |
| ATOM | 2512 | OH | TYR | 367 | 22.681 | 20.386 | 22.013 | 1.00 15.79 |
| ATOM | 2513 | C | TYR | 367 | 17.051 | 22.525 | 23.986 | 1.00 16.84 |
| MOTA | 2514 | ō | TYR | 367 | 17.918 | 23.063 | 24.688 | 1.00 17.12 |
| ATOM | 2514 | N | HIS | 368 | 16.467 | 23.141 | 22.965 | 1.00 17.12 |
| | | | | 368 | 16.831 | 24.511 | 22.611 | 1.00 17.01 |
| ATOM | 2516 2517 | CA | HIS | | | | | |
| ATOM | | CB | HIS | 368 | 16.277 | 24.847 | 21.220 | 1.00 18.64 |
| MOTA | 2518 | CG | HIS | 368 | 16.970 | 24.112 | 20.114 | 1.00 19.41 |
| MOTA | 2519 | | HIS | 368 | 16.608 | 23.014 | 19.409 | 1.00 19.84 |
| ATOM | 2520 | | HIS | 368 | 18.241 | 24.438 | 19.690 | 1.00 20.14 |
| ATOM | 2521 | | HIS | 368 | 18.633 | 23.570 | 18.775 | 1.00 20.20 |
| MOTA | 2522 | NE2 | HIS | 368 | 17.662 | 22.694 | 18.587 | 1.00 20.30 |
| MOTA | 2523 | C | HIS | 368 | 16.360 | 25.516 | 23.661 | 1.00 20.01 |
| MOTA | 2524 | 0 | HIS | 368 | 17.047 | 26.500 | 23.936 | 1.00 21.66 |
| MOTA | 2525 | N · | THR | 369 | 15.202 | 25.258 | 24.259 | 1.00 19.85 |
| ATOM | 2526 | CA | THR | 369 | 14.677 | 26.143 | 25.289 | 1.00 21.15 |
| ATOM | 2527 | CB | THR | 369 | 13.305 | 25.659 | 25.796 | 1.00 21.21 |
| ATOM | 2528 | OG1 | THR | 369 | 12.336 | 25.804 | 24.750 | 1.00 22.15 |
| ATOM | 2529 | CG2 | THR | 369 | 12.860 | 26.466 | 27.012 | 1.00 21.16 |
| ATOM | 2530 | С | THR | 369 | 15.634 | 26.241 | 26.474 | 1.00 22.56 |
| ATOM | 2531 | 0 | THR | 369 | 15.905 | 27.338 | 26.974 | 1.00 23.65 |
| ATOM | 2532 | N | ALA | 370 | 16.154 | 25.100 | 26.918 | 1.00 21.27 |
| ATOM | 2533 | CA | ALA | 370 | 17.078 | 25.078 | 28.051 | 1.00 23.22 |
| ATOM | 2534 | CB | ALA | 370 | 17.481 | 23.640 | 28.372 | 1.00 22.74 |
| ATOM | 2535 | C | ALA | 370 | 18.322 | 25.913 | 27.752 | 1.00 24.33 |
| ATOM | 2536 | 0 | ALA: | 370 | 18.775 | 26.694 | 28.593 | 1.00 24.36 |
| | | | | 371 | | | | 1.00 24.54 |
| ATOM | 2537 | N | ALA | | 18.862 | 25.744 26.480 | 26.548 | 1.00 24.34 |
| ATOM | 2538 | CA | ALA | 371 | 20.050 | | 26.115 | |
| ATOM | 2539 | CB | ALA | 371 | 20.465 | 26.019 | 24.719 | 1.00 24.54 |
| ATOM | 2540 | С | ALA | 371 | 19.795 | 27.986 | 26.109 | 1.00 27.22 |
| ATOM | 2541 | Ο. | ALA | 371 | 20.610 | 28.766 | 26.601 | 1.00 29.91 |
| ATOM | 2542 | N | VAL | 372 | 18.662 | 28.387 | 25.543 | 1.00 27.69 |
| MOTA | 2543 | CA | VAL | 372 | 18.299 | 29.796 | 25.473 | 1.00 28.62 |
| ATOM | 2544 | CB | VAL | 372 | 16.975 | 29.992 | 24.699 | 1.00 29.37 |
| MOTA | 2545 | CG1 | VAL | 372 | 16.541 | 31.448 | 24.749 | 1.00 28.12 |
| ATOM | 2546 | CG2 | VAL | 372 | 17.154 | 29.546 | 23.257 | 1.00 29.50 |
| MOTA | 2547 | С | VAL | 372 | 18.153 | 30.393 | 26.868 | 1.00 29.28 |
| MOTA | 2548 | 0 | VAL | 372 | 18.633 | 31.499 | 27.130 | 1.00 28.13 |
| MOTA | 2549 | N | ARG | 373 | 17.496 | 29.661 | 27.762 | 1.00 29.17 |
| ATOM | 2550 | CA | ARG | 373 | 17.299 | 30.138 | 29.128 | 1.00 29.87 |
| MOTA | 2551 | CB | ARG | 373 | 16.500 | 29.118 | 29.951 | 1.00 29.61 |
| MOTA | 2552 | CG | ARG | 373 | 16.378 | 29.474 | 31.437 | 1.00 29.17 |
| ATOM | 2553 | CD | ARG | 373 | 15.773 | 30.858 | 31.623 | 1.00 26.49 |
| MOTA | 2554 | NE | ARG | 373 | 14.370 | 30.903 | 31.228 | 1.00 28.14 |
| ATOM | 2555 | CZ | ARG | 373 | 13.703 | 32.022 | 30.961 | 1.00 27.87 |
| ATOM | 2556 | NH1 | | 373 | 14.307 | 33.199 | 31.042 | 1.00 27.29 |
| ATOM | 2557 | NH2 | | 373 | 12.427 | 31.967 | 30.614 | 1.00 28.85 |
| ATOM | 2558 | C | ARG | 373 | 18.630 | 30.415 | 29.811 | 1.00 31.14 |
| ATOM | 2559 | 0 | ARG | 373 | 18.763 | 31.394 | 30.547 | 1.00 31.14 |
| MOTA | 2560 | N | ARG | 374 | 19.615 | 29.554 | 29.573 | 1.00 32.05 |
| ATOM | 2561 | CA | | 374 | 20.928 | 29.743 | 30.175 | 1.00 32.05 |
| | | | ARG | | | | 29.798 | 1.00 34.00 |
| ATOM | 2562 | CB | ARG | 374 | 21.873 | 28.597 | | |
| ATOM | 2563 | CG | ARG | 374 | 21.388 | 27.221 | 30.202 | 1.00 33.93 |
| MOTA | 2564 | CD | ARG | 374 | 22.522 | 26.212 | 30.150 | 1.00 32.70 |
| MOTA | 2565 | NE | ARG | 374 | 22.071 | 24.854 | 30.450 | 1.00 33.93 |
| MOTA | 2566 | CZ | ARG | 374 | 21.510 | 24.033 | 29.565 | 1.00 33.76 |
| MOTA | 2567 | NH1 | | 374 | 21.329 | 24.423 | 28.311 | 1.00 30.05 |
| MOTA | 2568 | NH2 | | 374 | 21.131 | 22.817 | 29.936 | 1.00 33.89 |
| MOTA | 2569 | С | ARG | 374 | 21.532 | 31.066 | 29.713 | 1.00 34.72 |

| ATOM | 2570 | 0 | ARG | 374 | 22.160 | 31.780 | 30.496 | 1.00 36.00 |
|--------|------|-----|-----|-------|--------|--------|--------|------------|
| ATOM | 2571 | N | GLY | 375 | 21.331 | 31.388 | 28.439 | 1.00 35.42 |
| ATOM | 2572 | CA | GLY | 375 | 21.866 | 32.621 | 27.892 | 1.00 36.12 |
| ATOM | 2573 | C | GLY | 375 | 21.128 | 33.871 | 28.331 | 1.00 36.83 |
| ATOM | 2574 | 0 | GLY | 375 | 21.711 | 34.954 | 28.352 | 1.00 36.60 |
| ATOM | 2575 | N | ALA | 376 | 19.851 | 33.724 | 28.683 | 1.00 36.57 |
| ATOM | 2576 | CA | ALA | 376 | 19.027 | 34.851 | 29.114 | 1.00 37.33 |
| ATOM | 2577 | CB | ALA | 376 | 18.332 | 35.474 | 27.906 | 1.00 36.41 |
| ATOM | 2578 | C | ALA | 376 | 17.985 | 34.414 | 30.145 | 1.00 37.86 |
| ATOM | 2579 | 0 | ALA | 376 | 16.805 | 34.265 | 29.827 | 1.00 38.51 |
| ATOM | 2580 | N | PRO | 377 | 18.410 | 34.215 | 31.401 | 1.00 38.37 |
| ATOM | 2581 | CD | PRO | 377 | 19.789 | 34.359 | 31.901 | 1.00 38.55 |
| MOTA | 2582 | CA | PRO | 377 | 17.509 | 33.790 | 32.478 | 1.00 38.64 |
| MOTA | 2583 | CB | PRO | 377 | 18.474 | 33.389 | 33.586 | 1.00 39.17 |
| ATOM · | 2584 | CG | PRO | 377 | 19.588 | 34.359 | 33.404 | 1.00 38.79 |
| ATOM | 2585 | С | PRO | 377 | 16.513 | 34.851 | 32.936 | 1.00 38.71 |
| MOTA | 2586 | 0 | PRO | 377 | 15.691 | 34.596 | 33.814 | 1.00 38.56 |
| MOTA | 2587 | N | ASN | 378 | 16.580 | 36.033 | 32.334 | 1.00 38.88 |
| MOTA | 2588 | CA | ASN | 378 | 15.682 | 37.120 | 32.707 | 1.00 39.81 |
| ATOM | 2589 | CB | ASN | 378 | 16.490 | 38.288 | 33.279 | 1.00 41.15 |
| MOTA | 2590 | CG | ASN | 378 | 17.316 | 37.889 | 34.484 | 1.00 41.16 |
| ATOM | 2591 | OD1 | | 378 | 16.779 | 37.468 | 35.504 | 1.00 42.22 |
| MOTA | 2592 | ND2 | ASN | 378 | 18.632 | 38.018 | 34.369 | 1.00 43.85 |
| MOTA | 2593 | C | ASN | 378 | 14.838 | 37.613 | 31.540 | 1.00 39.91 |
| MOTA | 2594 | 0 | ASN | 378 | 14.375 | 38.754 | 31.541 | 1.00 42.79 |
| ATOM | 2595 | N | CYS | 379 | 14.635 | 36.763 | 30.541 | 1.00 38.30 |
| MOTA | 2596 | CA. | CYS | 379 | 13.843 | 37.164 | 29.383 | 1.00 36.58 |
| ATOM | 2597 | CB | CYS | 379 | 14.585 | 36.836 | 28.088 | 1.00 36.64 |
| ATOM | 2598 | SG | CYS | 379 | 14.422 | 35.102 | 27.558 | 1.00 37.37 |
| ATOM | 2599 | ·C | CYS | 379 | 12.494 | 36.460 | 29.355 | 1.00 34.98 |
| MOTA | 2600 | 0 | CYS | 379 | 12.290 | 35.465 | 30.039 | 1.00 35.06 |
| ATOM | 2601 | N | LEU | 380 | 11.576 | 37.002 | 28.565 | 1.00 33.89 |
| MOTA | 2602 | CA | LEU | 380 . | 10.261 | 36.411 | 28.397 | 1.00 32.87 |
| ATOM | 2603 | CB | LEU | 380 | 9.261 | 37.459 | 27.910 | 1.00 34.44 |
| ATOM | 2604 | CG | LEU | 380 | 7.810 | 36.999 | 27.743 | 1.00 34.49 |
| ATOM | 2605 | CD1 | LEU | 380 | 7.243 | 36.590 | 29.094 | 1.00 36.11 |
| ATOM | 2606 | CD2 | LEU | 380 | 6.982 | 38.120 | 27.139 | 1.00 36.04 |
| ATOM | 2607 | С | LEU | 380 | 10.485 | 35.353 | 27.319 | 1.00 32.33 |
| ATOM | 2608 | 0 | LEU | 380 | 10.675 | 35.686 | 26.147 | 1.00 31.37 |
| ATOM . | 2609 | N | LEU | 381 | 10.477 | 34.083 | 27.715 | 1.00 30.46 |
| MOTA | 2610 | CA | LEU | 381 | 10.726 | 32.994 | 26.775 | 1.00 28.43 |
| MOTA | 2611 | CB | LEU | 381 | 11.683 | 31.976 | 27.416 | 1.00 28.20 |
| MOTA | 2612 | CG | LEU | 381 | 12.577 | 31.092 | 26.539 | 1.00 29.26 |
| MOTA | 2613 | CD1 | LEU | 381 | 13.529 | 30.320 | 27.435 | 1.00 28.20 |
| MOTA | 2614 | CD2 | LEU | 381 - | 11.746 | 30.134 | 25.695 | 1.00 31.72 |
| ATOM | 2615 | C | LEU | 381 | 9.463 | 32.284 | 26.308 | 1.00 26.84 |
| MOTA | 2616 | 0 | LEU | 381 | 8.751 | 31.672 | 27.104 | 1.00 25.66 |
| ATOM | 2617 | N | LEU | 382 | 9.184 | 32.377 | 25.013 | 1.00 25.90 |
| MOTA | 2618 | CA | LEU | 382 | 8.026 | 31.706 | 24.436 | 1.00 26.12 |
| MOTA | 2619 | CB | LEU | 382 | 7.317 | 32.600 | 23.415 | 1.00 27.68 |
| ATOM | 2620 | CG | LEU | 382 | 6.383 | 33.685 | 23.955 | 1.00 29.10 |
| ATOM · | 2621 | CD1 | LEU | 382 | 7.172 | 34.713 | 24.751 | 1.00 29.94 |
| ATOM | 2622 | CD2 | LEU | 382 | 5.667 | 34.344 | 22.779 | 1.00 30.46 |
| MOTA | 2623 | С | LEU | 382 | 8.528 | 30.450 | 23.743 | 1.00 24.87 |
| ATOM | 2624 | 0 | LEU | 382 | 9.485 | 30.499 | 22.973 | 1.00 24.72 |
| ATOM | 2625 | N | ALA | 383 | 7.888 | 29.323 | 24.027 | 1.00 24.02 |
| MOTA | 2626 | CA | ALA | 383 | 8.286 | 28.060 | 23.422 | 1.00 22.33 |
| MOTA | | CB | ALA | 383 | 8.631 | 27.050 | 24.503 | 1.00 22.02 |
| ATOM | 2628 | С | ALA | 383 | 7.157 | 27.530 | 22.567 | 1.00 20.94 |
| ATOM | 2629 | 0 | ALA | 383 | 6.016 | 27.446 | 23.017 | 1.00 20.60 |
| ATOM | 2630 | N | ASP | 384 | 7.467 | 27.165 | 21.331 | 1.00 20.39 |
| MOTA | 2631 | CA | ASP | 384 | 6.440 | 26.631 | 20.448 | 1.00 20.57 |
| ATOM | 2632 | CB | ASP | 384 | 6.888 | 26.689 | 18.995 | 1.00 22.20 |
| ATOM | 2633 | CG | ASP | 384 | 6.278 | 27.847 | 18.232 | 1.00 24.06 |
| ATOM | 2634 | OD1 | | 384 | 5.235 | 28.372 | 18.661 | 1.00 26.53 |
| ATOM | 2635 | | ASP | 384 | 6.842 | 28.206 | 17.187 | 1.00 26.60 |
| ATOM | 2636 | C | ASP | 384 | 6.139 | 25.180 | 20.751 | 1.00 18.93 |
| MOTA | 2637 | 0 | ASP | 384 | 7.027 | 24.425 | 21.139 | 1.00 19.05 |
| ATOM | 2638 | N | LEU | 385 | 4.877 | 24.800 | 20.590 | 1.00 19.70 |
| ATOM | 2639 | CA | LEU | 3,85 | 4.504 | 23.398 | 20.725 | 1.00 19.65 |
| MOTA | 2640 | CB | LEU | 385 | 3.133 | 23.222 | 21.374 | 1.00 17.71 |
| MOTA | 2641 | CG | LEU | 385 | 3.087 | 23.370 | 22.901 | 1.00 16.98 |
| ATOM | 2642 | CD1 | | 385 | 1.716 | 22.965 | 23.429 | 1.00 15.13 |
| MOTA | 2643 | CD2 | | 385 | 4.162 | 22.498 | 23.523 | 1.00 16.02 |
| ATOM | 2644 | C | LEU | 385 | 4.462 | 23.012 | 19.246 | 1.00 20.97 |
| ATOM | 2645 | 0 | LEU | 385 | 3.705 | 23.596 | 18.461 | 1.00 21.82 |
| ATOM | 2646 | N | PRO | 386 | 5.303 | 22.047 | 18.841 | 1.00 19.88 |

| х пом | 2647 | CD | PRO | 386 | 6.168 | 21.273 | 19.747 | 1.00 20.26 |
|-------|------|------|-------|-------|---------|--------|--------|------------|
| MOTA | | | | | | | 17.466 | 1.00 19.86 |
| MOTA | 2648 | CA | PRO | 386 | 5.416 | 21.554 | | |
| MOTA | 2649 | CB | PRO | 386 | 6.626 | 20.633 | 17.537 | 1.00 21.72 |
| MOTA | 2650 | CG | PRO | 386 | 6.512 | 20.061 | 18.921 | 1.00 20.75 |
| MOTA | 2651 | С | PRO | 386 | 4.184 | 20.846 | 16.905 | 1.00 19.67 |
| ATOM | 2652 | 0 | PRO | 386 | 3.167 | 20.679 | 17.586 | 1.00 19.34 |
| ATOM | 2653 | N | PHE | 387 | 4.300 | 20.437 | 15.647 | 1.00 19.25 |
| ATOM | 2654 | CA | PHE | 387 | 3.248 | 19.739 | 14.927 | 1.00 18.90 |
| | | | PHE | 387 | 3.820 | 19.249 | 13.580 | 1.00 20.39 |
| MOTA | 2655 | CB | | | | | | |
| ATOM | 2656 | CG | PHE | 387 | 2.955 | 18.253 | 12.861 | 1.00 20.40 |
| MOTA | 2657 | CD1 | PHE | 387 | 1.653 | 18.573 | 12.479 | 1.00 21.35 |
| MOTA | 2658 | CD2 | PHE | 387 | 3.457 | 16.992 | 12.545 | 1.00 21.11 |
| MOTA | 2659 | CE1 | PHE | 387 | 0.863 | 17.651 | 11.789 | 1.00 22.07 |
| MOTA | 2660 | CE2 | PHE | 387 | 2.681 | 16.064 | 11.858 | 1.00 19.74 |
| ATOM | 2661 | CZ | PHE | 387 | 1.377 | 16.394 | 11.478 | 1.00 21.80 |
| ATOM | 2662 | C | PHE | 387 | 2.687 | 18.571 | 15.741 | 1.00 18.09 |
| | | | | 387 | 3.435 | 17.728 | 16.243 | 1.00 17.02 |
| MOTA | 2663 | 0 | PHE | | | | | |
| MOTA | 2664 | N | MET | 388 | 1.363 | 18.562 | 15.881 | 1.00 17.04 |
| ATOM | 2665 | CA | MET | 388 | 0.615 | 17.528 | 16.589 | 1.00 18.41 |
| ATOM | 2666 | CB | MET | 388 | 0.742 | 16.197 | 15.839 | 1.00 19.83 |
| MOTA | 2667 | CG | MET | 388 | -0.430 | 15.255 | 16.044 | 1.00 19.70 |
| MOTA | 2668 | SD | MET | 388 | -1.962 | 15.929 | 15.362 | 1.00 19.18 |
| ATOM | 2669 | CE | MET | 388 | -1.899 | 15.299 | 13.685 | 1.00 23.05 |
| ATOM | 2670 | C | MET | 388 | 0.986 | 17.332 | 18.062 | 1.00 18.34 |
| | | | | | 0.779 | | 18.622 | 1.00 10.54 |
| MOTA | 2671 | 0 | MET | 388 | | 16.254 | | |
| MOTA | 2672 | N | ALA | 389 | 1.520 | 18.376 | 18.688 | 1.00 17.11 |
| MOTA | 2673 | CA | ALA | 389 | 1.896 | 18.314 | 20.099 | 1.00 17.62 |
| MOTA | 2674 | CB | ALA - | 389 | 3.178 | 19.124 | 20.345 | 1.00 16.15 |
| MOTA | 2675 | С | ALA | 389 | 0.764 | 18.839 | 20.987 | 1.00 17.04 |
| MOTA | 2676 | 0 | ALA | 389 | 0.893 | 18.891 | 22.211 | 1.00 17.48 |
| ATOM | 2677 | N | TYR | 390 | -0.343 | 19.231 | 20.367 | 1.00 17.06 |
| ATOM | 2678 | CA | TYR | 390 | -1.496 | 19.727 | 21.111 | 1.00 18.54 |
| | | | | | -1.422 | 21.261 | 21.266 | 1.00 10.54 |
| MOTA | 2679 | CB | TYR | 390 | | | | |
| MOTA | 2680 | CG | TYR | 390 | -1.128 | 22.020 | 19.987 | 1.00 18.84 |
| ATOM | 2681 | CD1 | TYR | 390 | -2.157 | 22.468 | 19.157 | 1.00 21.00 |
| MOTA | 2682 | CE1 | TYR | 390 | -1.881 | 23.124 | 17.950 | 1.00 21.33 |
| ATOM | 2683 | .CD2 | TYR | 390 | 0.183 | 22.247 | 19.585 | 1.00 19.67 |
| ATOM | 2684 | CE2 | TYR | 390 | 0.471 | 22.895 | 18.390 | 1.00 22.68 |
| ATOM | 2685 | CZ | TYR | 390 | -0.566 | 23.329 | 17.579 | 1.00 21.64 |
| ATOM | 2686 | ОН | TYR | 390 | -0.262 | 23.963 | 16.394 | 1.00 23.80 |
| | | | | | | | | 1.00 23.00 |
| MOTA | 2687 | C | TYR | 390 | -2.790 | 19.291 | 20.437 | |
| MOTA | 2688 | 0 | TYR | 390 . | -3.765 | 20.039 | 20.376 | 1.00 18.45 |
| MOTA | 2689 | N | ALA | 391 | -2.780 | 18.050 | 19.949 | 1.00 18.00 |
| ATOM | 2690 | CA | ALA | 391 | -3.915 | 17.447 | 19.253 | 1.00 17.25 |
| MOTA | 2691 | CB | ALA | 391 | -3.497 | 16.109 | 18.656 | 1.00 18.23 |
| ATOM | 2692 | С | ALA | 391 | -5.112 | 17.258 | 20.177 | 1.00 17.88 |
| MOTA | 2693 | 0 | ALA | 391 | -6.250 | 17.147 | 19.719 | 1.00 18.08 |
| ATOM | 2694 | N | THR | 392 | -4.846 | 17.195 | 21.478 | 1.00 15.74 |
| ATOM | 2695 | CA | THR | 392 | -5.901· | 17.062 | 22.474 | 1.00 15.08 |
| | | | | | | | | |
| ATOM | 2696 | CB | THR | 392 | -6.124 | 15.605 | 22.917 | |
| MOTA | 2697 | OG1 | THR | 392 | -4.980 | 15.146 | 23.645 | 1.00 17.01 |
| MOTA | 2698 | CG2 | THR | 392 | -6.350 | 14.704 | 21.713 | 1.00 18.95 |
| ATOM | 2699 | C | THR | 392 | -5.445 | 17.857 | 23.682 | 1.00 14.74 |
| ATOM | 2700 | 0 | THR | 392 | -4.252 | 18.072 | 23.866 | 1.00 15.11 |
| ATOM | 2701 | N | PRO | 393 | -6.389 | 18.315 | 24.515 | 1.00 13.96 |
| ATOM | 2702 | CD | PRO | 393 | -7.851 | 18.291 | 24.353 | 1.00 15.31 |
| ATOM | 2703 | CA | PRO | 393 | -6.010 | 19.090 | 25.698 | 1.00 16.25 |
| ATOM | 2704 | CB | PRO | 393 | -7.349 | 19.309 | 26.398 | 1.00 15.99 |
| ATOM | 2704 | CG | PRO | 393 | -8.296 | 19.436 | 25.243 | 1.00 14.27 |
| | | | | | | | | |
| ATOM | 2706 | C | PRO | 393 | -5.016 | 18.320 | 26.550 | 1.00 16.25 |
| ATOM | 2707 | 0 | PRO | 393 | -3.983 | 18.855 | 26.964 | 1.00 16.74 |
| MOTA | 2708 | N | GLU | 394 | -5.323 | 17.049 | 26.781 | 1.00 17.06 |
| ATOM | 2709 | CA | GLU | 394 | -4.474 | 16.188 | 27.586 | 1.00 18.79 |
| ATOM | 2710 | CB | GLU | 394 | -5.044 | 14.771 | 27.591 | 1.00 22.17 |
| ATOM | 2711 | CG | GLU | 394 | -4.455 | 13.860 | 28.630 | 1.00 29.13 |
| ATOM | 2712 | CD | GLU | 394 | -5.105 | 12.495 | 28.613 | 1.00 33.05 |
| ATOM | 2713 | | GLU | 394 | -4.687 | 11.644 | 27797 | 1.00 35.69 |
| | | | | | -6.055 | 12.288 | | 1.00 33.03 |
| ATOM | 2714 | | GLU | 394 | | | 29.402 | |
| ATOM | 2715 | C | GLU | 394 | -3.029 | 16.167 | 27.088 | 1.00 17.93 |
| ATOM | 2716 | 0 | GLU | 394 | -2.092 | 16.296 | 27.878 | 1.00 17.60 |
| MOTA | 2717 | N | GLN | 395 | -2.832 | 16.002 | 25.783 | 1.00 16.16 |
| ATOM | 2718 | CA | GLN | 395 | -1.469 | 15.973 | 25.261 | 1.00 18.13 |
| MOTA | 2719 | CB | GLN | 395 | -1.451 | 15.465 | 23.819 | 1.00 19.78 |
| ATOM | 2720 | CG | GLN | 395 | -1.662 | 13.958 | 23.738 | 1.00 26.51 |
| ATOM | 2721 | CD | GLN | 395 | -1.756 | 13.447 | 22.320 | 1.00 27.20 |
| ATOM | 2722 | | GLN | 395 | -0.821 | 13.590 | 21.535 | 1.00 31.74 |
| ATOM | | | GLN | 395 | -2.889 | 12.836 | 21.986 | 1.00 31.74 |
| ATOM | 2723 | NEZ | GLIM | 393 | -2.009 | 12.030 | 21.300 | 1.00 31.10 |
| | | | | | | | | |

| ATOM | 2724 | С | GLN | 395 | -0.812 | 17.342 | 25.348 | 1.00 16.31 |
|--------|-------|------|-------|-----|--------|--------|--------|------------|
| ATOM | 2725 | 0 | GLN | 395 | 0.394 | 17.448 | 25.560 | 1.00 15.19 |
| ATOM | 2726 | N | ALA | 396 | -1.611 | 18.389 | 25.172 | 1.00 15.71 |
| ATOM | 2727 | CA | ALA | 396 | -1.097 | 19.748 | 25.258 | 1.00 15.45 |
| MOTA | 2728 | CB | ALA | 396 | -2.203 | 20.754 | 24.941 | 1.00 14.95 |
| MOTA | 2729 | С | ALA | 396 | -0.552 | 19.995 | 26.665 | 1.00 15.89 |
| ATOM | 2730 | 0 | ALA | 396 | 0.535 | 20.548 | 26.832 | 1.00 15.31 |
| MOTA | 2731 | N | PHE | 397 | -1.306 | 19.581 | 27.679 | 1.00 17.14 |
| ATOM | 2732 | CA | PHE | 397 | -0.862 | 19.780 | 29.059 | 1.00 17.67 |
| MOTA | 2733 | CB | PHE | 397 | -1.855 | 19.179 | 30.062 | 1.00 17.74 |
| MOTA | 2734 | CG | PHE | 397 | -3.276 | 19.626 | 29.876 | 1.00 15.92 |
| ATOM | 2735 | CD1 | PHE | 397 | -3.571 | 20.887 | 29.368 | 1.00 17.98 |
| ATOM | 2736 | CD2 | PHE | 397 | -4.325 | 18.787 | 30.242 | 1.00 18.15 |
| ATOM | 2737 | CE1 | PHE | 397 | -4.891 | 21.311 | 29.222 | 1.00 20.21 |
| ATOM | 2738 | CE2 | PHE | 397 | -5.650 | 19.197 | 30.103 | 1.00 19.30 |
| ATOM | 2739 | CZ | PHE | 397 | -5.934 | 20.465 | 29.591 | 1.00 20.13 |
| MOTA | 2740 | С | PHE | 397 | 0.496 | 19.120 | 29.277 | 1.00 17.87 |
| MOTA | 2741 | 0 | PHE | 397 | 1.397 | 19.710 | 29.867 | 1.00 18.64 |
| MOTA | 2742 | N | GLU | 398 | 0.628 | 17.887 | 28.793 | 1.00 18.39 |
| ATOM | 2743 | CA | GLU | 398 | 1.853 | 17.109 | 28.942 | 1.00 19.60 |
| MOTA | 2744 | CB | GLU | 398 | 1.612 | 15.691 | 28.411 | 1.00 22.86 |
| MOTA | 2745 | CG | GLU | 398 | 2.689 | 14.663 | 28.722 | 1.00 27.33 |
| ATOM | 2746 | CD | GLU | 398 | 2.800 | 14.340 | 30.203 | 1.00 31.00 |
| MOTA | 2747 | OE1 | GLU | 398 | 1.840 | 14.603 | 30.958 | 1.00 32.52 |
| MOTA | 2748 | OE2 | GLU | 398 | 3.854 | 13.804 | 30.606 | 1.00 34.89 |
| MOTA | 2749 | С | GLU | 398 | 3.047 | 17.740 | 28.224 | 1.00 17.86 |
| MOTA | 2750 | 0 | GLU. | 398 | 4.139 | 17.864 | 28.791 | 1.00 17.51 |
| MOTA | 2751 | N | ASN · | 399 | 2.836 | 18.143 | 26.977 | 1.00 17.52 |
| MOTA | 2752 | CA | ASN | 399 | 3.903 | 18.750 | 26.184 | 1.00 17.00 |
| ATOM | 2753 | CB | ASN | 399 | 3.545 | 18.695 | 24.696 | 1.00 17.91 |
| MOTA | 2754 | CG | ASN | 399 | 3.554 | 17.274 | 24.171 | 1.00 17.94 |
| MOTA | 2755 | OD1 | ASN | 399 | 4.421 | 16.482 | 24.557 | 1.00 16.74 |
| MOTA | 2756 | ND2 | ASN | 399 | 2.614 | 16.939 | 23.297 | 1.00 14.86 |
| MOTA | 2757 | С | ASN | 399 | 4.248 | 20.174 | 26.598 | 1.00 16.90 |
| MOTA | 2758 | 0 | ASN | 399 | 5.426 | 20.560 | 26.582 | 1.00 14.68 |
| MOTA | 2759 | N | ALA | 400 | 3.231 | 20.958 | 26.953 | 1.00 17.41 |
| MOTA | 2760 | CA | ALA | 400 | 3.465 | 22.324 | 27.403 | 1.00 17.58 |
| MOTA | 2761 | CB | ALA | 400 | 2.136 | 23.038 | 27.668 | 1.00 17.90 |
| ATOM | 2762 | С | ALA | 400 | 4.272 | 22.249 | 28.694 | 1.00 17.52 |
| MOTA | 2763 | 0 : | ALA | 400 | 5.199 | 23.028 | 28.902 | 1.00 18.40 |
| MOTA | 2764 | N | ALA | 401 | 3.925 | 21.298 | 29.558 | 1.00 18.00 |
| MOTA | 2765 | CA | ALA | 401 | 4.629 | 21.152 | 30.825 | 1.00 17.86 |
| ATOM | 2766 | CB | ALA | 401 | 3.953 | 20.085 | 31.698 | 1.00 17.24 |
| MOTA | 2767 | C | ALA | 401 | 6.087 | 20.800 | 30.599 | 1.00 17.50 |
| MOTA | 2768 | 0 | ALA | 401 | 6.966 | 21.243 | 31.341 | 1.00 17.32 |
| ATOM | 2769 | N | THR | 402 | 6.349 | 20.004 | 29.569 | 1.00 17.75 |
| MOTA | 2770 | CA | THR | 402 | 7.714 | 19.604 | 29.259 | 1.00 17.20 |
| MOTA | 2771 | CB | THR | 402 | 7.744 | 18.579 | 28.100 | 1.00 17.19 |
| MOTA | 2772 | OG1 | THR | 402 | 7,194 | 17.332 | 28.551 | 1.00 15.26 |
| ATOM | 2773 | CG2 | THR | 402 | 9.169 | 18.361 | 27.621 | 1.00 17.10 |
| MOTA | 2774 | С | THR | 402 | 8.576 | 20.807 | 28.883 | 1.00 18.60 |
| MOTA | 2775 | 0 | THR | 402 | 9.690 | 20.954 | 29.380 | 1.00 18.32 |
| ATOM . | 2776 | N | VAL | 403 | 8.063 | 21.675 | 28.016 | 1.00 18.13 |
| MOTA | 2777 | CA | VAL | 403 | 8.845 | 22.830 | 27.603 | 1.00 19.86 |
| MOTA | 2778 | CB | VAL | 403 | 8.313 | 23.416 | 26.275 | 1.00 20.58 |
| ATOM | 2779 | CG1 | | 403 | 9.411 | 24.207 | 25.600 | 1.00 25.39 |
| ATOM | 278.0 | CG2 | VAL | 403 | 7.857 | 22.290 | 25.344 | 1.00 22.84 |
| ATOM | 2781 | С | VAL | 403 | 8.886 | 23.901 | 28.702 | 1.00 21.59 |
| ATOM | 2782 | 0 | VAL | 403 | 9.825 | 24.701 | 28.769 | 1.00 21.71 |
| ATOM | 2783 | N | MET | 404 | 7.870 | 23.909 | 29.563 | 1.00 21.27 |
| ATOM | 2784 | CA | MET | 404 | 7.819 | 24.849 | 30.682 | 1.00 23.55 |
| ATOM | 2785 | CB | MET | 404 | 6.442 | 24.813 | 31.354 | 1.00 26.11 |
| MOTA | 2786 | CG | MET | 404 | 5.312 | 25.363 | 30.498 | 1.00 30.04 |
| ATOM. | 2787 | SD | MET | 404 | 5.514 | 27.112 | 30.150 | 1.00 34.43 |
| MOTA | 2788 | CE | MET | 404 | 4.846 | 27.830 | 31.675 | 1.00 33.59 |
| MOTA | 2789 | C | MET | 404 | 8.902 | 24.474 | 31.704 | 1.00 22.56 |
| MOTA | 2790 | 0 | MET | 404 | 9.649 | 25.335 | 32.168 | 1.00 23.06 |
| ATOM | 2791 | N | ARG | 405 | 8.988 | 23.190 | 32.053 | 1.00 20.96 |
| MOTA | 2792 | CA | ARG | 405 | 9.998 | 22.739 | 33.008 | 1.00 21.29 |
| MOTA | 2793 | CB | ARG | 405 | 9.816 | 21.254 | 33.365 | 1.00 19.72 |
| ATOM | 2794 | CG | ARG | 405 | 8.471 | 20.900 | 33.973 | 1.00 19.05 |
| ATOM | 2795 | CD | ARG | 405 | 8.506 | 19.570 | 34.721 | 1.00 18.65 |
| ATOM | 2796 | NE | ARG | 405 | 7.157 | 19.145 | 35.096 | 1.00 22.57 |
| ATOM | 2797 | CZ · | ARG | 405 | 6.330 | 18.474 | 34.299 | 1.00 21.33 |
| ATOM | 2798 | NH1 | | 405 | 6.717 | 18.130 | 33.075 | 1.00 23.18 |
| ATOM | 2799 | NH2 | | 405 | 5.101 | 18.180 | 34.709 | 1.00 20.27 |
| MOTA | 2800 | С | ARG | 405 | 11.395 | 22.948 | 32.419 | 1.00 21.30 |

| MOTA | 2801 | 0 | ARG | 405 | 12.385 | 23.004 | 33.144 | 1.00 | 20.18 |
|--------------|--------------|-----------|------------|------------|----------------|------------------|------------------|------|--------------------|
| MOTA | 2802 | N | ALA | 406 | 11.465 | 23.068 | 31.097 | 1.00 | 21.02 |
| MOTA | 2803 | CA | ALA | 406 | 12.734 | 23.272 | 30.421 | 1.00 | 21.90 |
| MOTA | 2804 | CB | ALA | 406 | 12.625 | 22.844 | 28.961 | 1.00 | 22.53 |
| MOTA | 2805 | С | ALA | 406 | 13.188 | 24.730 | 30.511 | 1.00 | 24.17 |
| MOTA | 2806 | 0 | ALA | 406 | 14.331 | 25.050 | 30.182 | 1.00 | 24.00 |
| MOTA | 2807 | N | GLY | 407 | 12.298 | 25.616 | 30.950 | 1.00 | 24.29 |
| MOTA | 2808 | CA | GLY | 407 | 12.671 | 27.017 | 31.083 | 1.00 | 27.67 |
| MOTA | 2809 | С | GLY | 407 | 11.739 | 28.021 | 30.429 | 1.00 | 27.96 |
| MOTA | 2810 | 0 | GLY | 407 | 11.841 | 29.225 | 30.672 | | 27.55 |
| MOTA | 2811 | N | ALA | 408 | 10.827 | 27.536 | 29.595 | 1.00 | 28.22 |
| ATOM · | 2812 | CA | ALA | 408 | 9.892 | 28.423 | 28.920 | | 27.88 |
| MOTA | 2813 | CB | ALA | 408 | 9.114 | 27.654 | 27.861 | | 29.62 |
| MOTA | 2814 | С | ALA | 408 | 8.928 | 29.058 | 29.915 | 1.00 | 28.28 |
| ATOM | 2815 | | ALA | 408 | 8.602 | 28.462 | 30.944 | 1.00 | 27.83 |
| ATOM | 2816 | N | ASN | 409 | 8.480 | 30.271 | 29.602 | 1.00 | 27.03 |
| ATOM | 2817 | CA | ASN | 409 | 7.539 | 30.996 | 30.454 | | 27.18 29.08 |
| ATOM | 2818 | CB | ASN | 409 409 | 7.971 9.327 | 32.453 32.590 | 30.632 31.274 | | 28.79 |
| ATOM ATOM | 2819 2820 | CG OD1 | ASN ASN | 409 | 9.552 | 32.390 | 32.394 | 1.00 | 28.82 |
| ATOM | 2821 | ND2 | | 409 | 10.245 | 33.244 | 30.571 | | 27.34 |
| ATOM | 2822 | C | ASN | 409 | 6.156 | 30.993 | 29.823 | | 26.67 |
| ATOM | 2823 | Ö | ASN | 409 | 5.150 | 31.201 | 30.501 | | 25.46 |
| ATOM | 2824 | N | MET | 410 | 6.114 | 30.767 | 28.515 | | 24.91 |
| ATOM | 2825 | CA | MET | 410 | 4.853 | 30.758 | 27.781 | | 24.64 |
| ATOM | 2826 | CB | MET | 410 | 4.549 | 32.173 | 27.279 | | 26.21 |
| ATOM | 2827 | CG | MET | 410 | 3.244 | 32.339 | 26.516 | 1.00 | 28.39 |
| ATOM | 2828 | SD | MET | 410 | 3.036 | 34.056 | 25.925 | | 30.91 |
| ATOM | 2829 | CE | MET | 410 | 1.737 | 34.676 | 27.032 | | 31.25 |
| ATOM | 2830 | С | MET | 410 | 4.947 | 29.794 | 26.605 | 1.00 | 23.26 |
| MOTA | 2831 | 0 | MET | 410 | 6.039 | 29.499 | 26.125 | 1.00 | 21.44 |
| ATOM | 2832 | N | VAL | 411 | 3.796 | 29.313 | 26.151 | 1.00 | 22.20 |
| MOTA | 2833 | CA | VAL | 411 | 3.726 | 28.381 | 25.035 | 1.00 | 24.32 |
| ATOM . | 2834 | CB | VAL | 411 | 3.045 | 27.060 | 25.482 | | 25.61 |
| MOTA | 2835 | | VAL | 411 | 2.625 | 26.248 | 24.281 | | 30.37 |
| MOTA | 2836 | | VAL | 411 | 3.998 | 26.257 | 26.354 | | 25.91 |
| MOTA | 2837 | C . | VAL | 411 | 2.930 | 28.978 | 23.875 | | 23.06 |
| ATOM | 2838 | 0 | VAL | 411 | 1.933 | 29.670 | 24.087 | 1.00 | 23.99 |
| MOTA | 2839 | N | LYS | 412 | 3.372 | 28.714 | 22.649 | 1.00 | |
| ATOM | 2840 | CA | LYS | 412 | 2.674 | 29.220 | 21.471 | 1.00 | 22.52 |
| ATOM | 2841 | CB | LYS | 412 412 | 3.616 2.927 | 30.080 30.727 | 20.611 19.405 | 1.00 | |
| ATOM ATOM | 2842 2843 | CG CD | LYS LYS | 412 | 3.725 | 31.898 | 18.838 | | 22.53 |
| ATOM | 2844 | CE | LYS | 412 | 4.979 | 31.436 | 18.103 | | 22.01 |
| ATOM | 2845 | NZ | LYS | 412 | 4.638 | 30.645 | 16.892 | 1.00 | 20.94 |
| ATOM | 2846 | C | LYS | 412 | 2.129 | 28.056 | 20.649 | 1.00 | |
| ATOM | 2847 | ō | LYS | 412 | 2.830 | 27.071 | 20.406 | 1.00 | |
| ATOM | 2848 | N | ILE | 413 | 0.870 | 28.170 | 20.240 | 1.00 | |
| ATOM | 2849 | CA | ILE | 413 | 0.212 | 27.138 | 19.437 | 1.00 | 26.66 |
| ATOM | 2850 | CB | ILE | 413 | -0.758 | 26.291 | 20.295 | 1.00 | 26.12 |
| ATOM | 2851 | CG2 | ILE | 413 | 0.028 | 25.460 | 21.299 | 1.00 | 26.91 |
| MOTA | . 2852 | CG1 | ILE | 413 | -1.751 | 27.203 | 21.020 | 1.00 | 28.28 |
| MOTA | 2853 | CD1 | ILE | 413 | -2.796 | 26.446 | 21.830 | | 24.14 |
| MOTA | 2854 | С | ILE | 413 | -0.580 | 27.747 | 18.282 | | 27.66 |
| MOTA | 2855 | 0 | ILE | 413 | -1.152 | 28.829 | 18.414 | | 28.22 |
| ATOM | 2856 | N | GLU | 414 | -0.615 | 27.037 | 17.158 | | 29.05 |
| ATOM | 2857 | CA | GLU | 414 | -1.318 | 27.489 | 15.958 | | 30.52 |
| ATOM | 2858 | CB | GLU | 414 | -0.569 | 27.025 | 14.707 | | 31.51 |
| MOTA | 2859 | CG | GLU | 414 | 0.834 | 27.574 | 14.561 13.416 | | 32.37 |
| ATOM | 2860 | CD | GLU | 414 | 1.593 0.951 | 26.923 26.261 | 12.568 | | 32.40 |
| ATOM ATOM | 2861 2862 | OE2 | GLU GLU | 414 414 | 2.832 | 27.082 | 13.356 | | 32.46 |
| MOTA | 2863 | C | GLU | 414 | -2.743 | 26.961 | 15.887 | | 32.40 |
| ATOM | 2864 | 0 | GLU | 414 | -2.997 | 25.800 | 16.201 | | 33.94 |
| ATOM . | 2865 | N | GLY | 415 | -3.672 | 27.809 | 15.458 | | 32.73 |
| ATOM | 2866 | CA | GLY | 415 | -5.052 | 27.372 | 15.345 | | 33.14 |
| ATOM | 2867 | C | GLY | 415 | -6.074 | 28.431 | 15.703 | | 32.54 |
| ATOM | 2868 | ō | GLY | 415 | -5.744 | 29.432 | 16.336 | | 31.25 |
| MOTA | 2869 | N | GLY | 416 | -7.322 | 28.199 | 15.302 | | 33.53 |
| MOTA | 2870 | CA | GLY | 416 | -8.386 | 29.148 | 15.586 | | 34.28 |
| ATOM | 2871 | С | GLY | 416 | -9.369 | 28.688 | 16.650 | 1.00 | 35.11 ⁻ |
| MOTA | 2872 | 0 | GLY | 416 | -8.976 | 28.275 | 17.741 | | 35.72 |
| MOTA | 2873 | N | GLU . | 417 | -10.656 | 28.762 | 16.324 | | 34.22 |
| MOTA | 2874 | CA | GLU | 417 | -11.723 | 28.370 | 17.240 | | 34.97 |
| MOTA | 2875 | CB | GLU | 417 | -13.076 | 28.448 | 16.527 | | 38.06 |
| ATOM | 2876 | CG | GLU | 417 | -13.709 | 29.829 | 16.530 | | 44.07 |
| MOTA | 2877 | CD | GLU | 417 | -14.416 | 30.149 | 17.835 | 1.00 | 46.62 |

| MOTA | 2878 | OE1 | GLU | 417 | -13.763 | 30.094 | 18.900 | 1.00 48.75 |
|------|--------|-----|-----|-------|---------|--------|--------|------------|
| ATOM | 2879 | OE2 | GLU | 417 | -15.628 | 30.457 | 17.793 | 1.00 48.44 |
| | 2880 | C | GLU | 417 | -11.576 | 26.986 | 17.861 | 1.00 33.06 |
| MOTA | | | | | | | 19.008 | 1.00 31.36 |
| ATOM | 2881 | 0 | GLU | 417 | -11.974 | 26.778 | | |
| MOTA | 2882 | N | TRP | 418 | -11.011 | 26.041 | 17.115 | 1.00 31.17 |
| MOTA | 2883 | CA | TRP | 418 | -10.865 | 24.683 | 17.632 | 1.00 30.62 |
| MOTA | 2884 | CB | TRP | 418 | -10.427 | 23.710 | 16.526 | 1.00 29.57 |
| ATOM | 2885 | CG | TRP | 418 | -8.968 | 23.794 | 16.161 | 1.00 27.67 |
| ATOM | 2886 | CD2 | TRP | 418 | -7.909 | 22.968 | 16.666 | 1.00 27.03 |
| , | | | | | | | 16.063 | 1.00 25.39 |
| MOTA | 2887 | CE2 | TRP | 418 | -6.710 | 23.410 | | |
| MOTA | 2888 | CE3 | TRP | 418 | -7.856 | 21.901 | 17.575 | 1.00 25.44 |
| MOTA | 2889 | CD1 | TRP | 418 | -8.386 | 24.674 | 15.297 | 1.00 27.61 |
| ATOM | 2890 | NE1 | TRP | 418 | -7.030 | 24.449 | 15.231 | 1.00 25.85 |
| MOTA | 2891 | CZ2 | TRP | 418 | -5.471 | 22.817 | 16.333 | 1.00 24.66 |
| ATOM | 2892 | CZ3 | TRP | 418 | -6.618 | 21.313 | 17.843 | 1.00 24.48 |
| ATOM | 2893 | CH2 | TRP | 418 | -5.446 | 21.777 | 17.225 | 1.00 24.32 |
| | | | TRP | 418 | -9.900 | 24.568 | 18.810 | 1.00 29.99 |
| MOTA | 2894 | С | | | | | | |
| MOTA | 2895 | 0 | TRP | 418 | -9.793 | 23.500 | 19.417 | 1.00 31.23 |
| ATOM | 2896 | N | LEU | 419 | -9.208 | 25.661 | 19.131 | 1.00 26.75 |
| MOTA | 2897 | CA | LEU | 419 | -8.244 | 25.677 | 20.235 | 1.00 26.72 |
| MOTA | 2898 | CB | LEU | 419 | -6.950 | 26.371 | 19.809 | 1.00 25.59 |
| ATOM | 2899 | CG | LEU | 419 | -6.010 | 25.613 | 18.872 | 1.00 26.52 |
| ATOM | 2900 | | LEU | 419 | -4.746 | 26.434 | 18.644 | 1.00 25.61 |
| | 2901 | | LEU | | -5.659 | 24.268 | 19.488 | 1.00 23.92 |
| ATOM | | | | 419 | | | | |
| MOTA | 2902 | С | LEU | 419 | -8.755 | 26.355 | 21.498 | 1.00 26.45 |
| MOTA | 2903 | 0 | LEU | 419 | -8.051 | 26.412 | 22.507 | 1.00 23.45 |
| ATOM | 2904 | N | VAL | 420 | -9.976 | 26.871 | 21.442 | 1.00 25.42 |
| ATOM | 2905 | CA | VAL | 420 | -10.562 | 27.544 | 22.591 | 1.00 25.27 |
| ATOM | 2906 | CB | VAL | 420 | -12.053 | 27.865 | 22.340 | 1.00 25.27 |
| ATOM | 2907 | | VAL | 420 | -12.701 | 28.408 | 23.619 | 1.00 25.70 |
| ATOM | | CG2 | | 420 | -12.171 | 28.891 | 21.220 | 1.00 25.05 |
| | 2908 | | | | | | | |
| ATOM | 2909 | C | VAL | 420 | -10.434 | 26.701 | 23.857 | 1.00 24.44 |
| MOTA | 2910 | 0 | VAL | 420 | -9.785 | 27,109 | 24.819 | 1.00 24.50 |
| ATOM | 2911 | N | GLU | 421 | -11.041 | 25.520 | 23.842 | 1.00 23.25 |
| MOTA | 2912 | CA | GLU | 421 | -11.000 | 24.635 | 24.999 | 1.00 23.68 |
| MOTA | 2913 | CB | GLU | 421 | -11.659 | 23.301 | 24.654 | 1.00 26.62 |
| ATOM | 2914 | CG | GLU | 421 | -11.745 | 22.350 | 25.825 | 1.00 30.68 |
| ATOM | 2915 | CD | GLU | 421 | -12.603 | 21.141 | 25.526 | 1.00 32.30 |
| | | | | | | | | |
| ATOM | 2916 | | GLU | 421 | -12.199 | 20.308 | 24.688 | |
| MOTA | 2917 | OE2 | GLU | 421 | -13.692 | 21.036 | 26.129 | 1.00 36.59 |
| MOTA | 2918 | C | GLU | 421 | -9.576 | 24.393 | 25.513 | 1.00 22.94 |
| MOTA | 2919 | 0 | GLU | 421 | -9.320 | 24.490 | 26.711 | 1.00 21.48 |
| MOTA | 2920 | N | THR | 422 | -8.660 | 24.079 | 24.602 | 1.00 21.94 |
| ATOM | 2921 | CA | THR | 422 | -7.267 | 23.827 | 24.952 | 1.00 20.34 |
| ATOM | 2922 | CB | THR | 422 - | -6.456 | 23.462 | 23.692 | 1.00 21.24 |
| | 2923 | | | 422 | -7.015 | 22.283 | 23.103 | 1.00 20.48 |
| ATOM | | OG1 | THR | | | | | |
| ATOM | 2924 | CG2 | THR | 422 | -4.991 | 23.211 | 24.032 | 1.00 19.54 |
| MOTA | 2925 | С | THR | 422 | -6.634 | 25.042 | 25.625 | 1.00 21.57 |
| MOTA | . 2926 | 0 | THR | 422 | -5.871 | 24.916 | 26.591 | 1.00 20.08 |
| ATOM | 2927 | N | VAL | 423 | -6.951 | 26.224 | 25.109 | 1.00 22.38 |
| MOTA | 2928 | CA | VAL | 423 | -6.420 | 27.453 | 25.675 | 1.00 23.54 |
| MOTA | 2929 | СВ | VAL | 423 | -6.755 | 28.672 | 24.794 | 1.00 24.18 |
| ATOM | 2930 | | VAL | 423 | -6.307 | 29.955 | 25.497 | 1.00 24.10 |
| ATOM | 2931 | | VAL | 423 | -6.064 | 28.540 | 23.455 | 1.00 22.31 |
| | | | | | | | | 1.00 24.57 |
| ATOM | 2932 | C | VAL | 423 | -6.973 | 27.699 | 27.074 | |
| ATOM | 2933 | 0 | VAL | 423 | -6.221 | 28.014 | 27.994 | 1.00 24.45 |
| MOTA | 2934 | N | GLN | 424 | -8.286 | 27.554 | 27.231 | 1.00 24.53 |
| MOTA | 2935 | CA | GLN | 424 | -8.910 | 27.776 | 28.529 | 1.00 25.29 |
| MOTA | 2936 | CB | GLN | 424 | -10.429 | 27.587 | 28.438 | 1.00 26.08 |
| MOTA | 2937 | CG | GLN | 424 | -11.088 | 28.337 | 27.289 | 1.00 29.30 |
| ATOM | 2938 | CD | GLN | 424 | -12.604 | 28.243 | 27.319 | 1.00 31.02 |
| ATOM | 2939 | OE1 | | 424 | -13.171 | 27.155 | 27.423 | 1.00 27.95 |
| | | | | | -13.269 | 29.390 | 27.220 | 1.00 27.33 |
| ATOM | 2940 | NE2 | | 424 | | | | |
| ATOM | 2941 | С | GLN | 424 | -8.338 | 26.819 | 29.568 | 1.00 25.02 |
| MOTA | 2942 | 0 | GLN | 424 | -7.998 | 27.225 | 30.677 | 1.00 23.19 |
| MOTA | 2943 | N | MET | 425 | -8.216 | 25.549 | 29.204 | 1.00 21.87 |
| MOTA | 2944 | CA | MET | 425 | -7.703 | 24.556 | 30.135 | 1.00 22.36 |
| MOTA | 2945 | CB | MET | 425 | -8.003 | 23.155 | 29.609 | 1.00 22.27 |
| ATOM | 2946 | CG | MET | 425 | -9.484 | 22.889 | 29.484 | 1.00 23.95 |
| ATOM | 2947 | SD | MET | 425 | -9.848 | 21.203 | 29.002 | 1.00 24.90 |
| | | | | | | | | |
| ATOM | 2948 | CE | MET | 425 | -9.831 | 20.377 | 30.583 | 1.00 28.11 |
| ATOM | 2949 | С | MET | 425 | -6.216 | 24.707 | 30.448 | 1.00 20.61 |
| MOTA | 2950 | 0 | MET | 425 | -5.791 | 24.450 | 31.571 | 1.00 20.01 |
| MOTA | 2951 | N | LEU | 426 | -5.426 | 25.122 | 29.463 | 1.00 20.23 |
| MOTA | 2952 | CA | LEU | 426 | -3.999 | 25.315 | 29.685 | 1.00 20.83 |
| MOTA | 2953 | СВ | LEU | 426 | -3.291 | 25.634 | | 1.00 18.83 |
| ATOM | 2954 | CG | LEU | 426 | -2.789 | 24.412 | 27.576 | 1.00 16.82 |
| | | | | | , | | | 20.00 |
| | | | | | | | | |

| ATOM | 2955 | CD1 | LEU | 426 | -2.321 | 24.828 | 26.188 | 1.00 18.65 |
|--------|------|-----|----------------------|-----|---------|--------|--------|------------|
| ATOM | 2956 | CD2 | LEU | 426 | -1.642 | 23.764 | 28.344 | 1.00 18.65 |
| ATOM | 2957 | С | LEU | 426 | -3.810 | 26.465 | 30.668 | 1.00 24.13 |
| ATOM | 2958 | ō | LEU | 426 | -2.952 | 26.411 | 31.550 | 1.00 23.47 |
| ATOM | 2959 | N | THR | 427 | -4.631 | 27.498 | 30.505 | 1.00 27.30 |
| ATOM | 2960 | CA | THR | 427 | -4.594 | 28.681 | 31.357 | 1.00 31.01 |
| | | | | 427 | -5.694 | | 30.957 | 1.00 31.69 |
| MOTA | 2961 | CB | THR | | | 29.685 | | 1.00 31.09 |
| MOTA | 2962 | | THR | 427 | -5.486 | 30.107 | 29.605 | |
| ATOM | 2963 | CG2 | | 427 | -5.665 | 30.903 | 31.868 | 1.00 34.25 |
| ATOM | 2964 | С | THR | 427 | -4.774 | 28.340 | 32.831 | 1.00 31.38 |
| ATOM | 2965 | 0 | THR | 427 | -3.902 | 28.627 | 33.646 | 1.00 31.24 |
| ATOM | 2966 | N | GLU | 428 | -5.905 | 27.727 | 33.172 | 1.00 32.66 |
| MOTA | 2967 | CA | GLU | 428 | -6.168 | 27.375 | 34.563 | 1.00 32.58 |
| ATOM | 2968 | CB. | GLU | 428 | -7.614 | 26.899 | 34.741 | 1.00 33.84 |
| MOTA | 2969 | CG | GLU | 428 | -8.107 | 25.949 | 33.673 | 1.00 34.13 |
| ATOM | 2970 | CD | GLU | 428 | -9.482 | 25.377 | 33.995 | 1.00 34.03 |
| MOTA | 2971 | OE1 | GLU | 428 | -10.368 | 26.145 | 34.438 | 1.00 30.96 |
| MOTA | 2972 | | GLU | 428 | -9.673 | 24.162 | 33.793 | 1.00 31.63 |
| ATOM | 2973 | C | GLU | 428 | -5.206 | 26.339 | 35.134 | 1.00 32.23 |
| ATOM | 2974 | ō | GLU | 428 | -5.269 | 26.022 | 36.320 | 1.00 32.97 |
| ATOM | 2975 | N | ARG | 429 | -4.314 | 25.816 | 34.296 | 1.00 31.00 |
| ATOM | 2976 | CA | ARG | 429 | -3.339 | 24.831 | 34.753 | 1.00 27.80 |
| | | | ARG | 429 | -3.372 | 23.594 | 33.844 | 1.00 27.60 |
| ATOM | 2977 | CB | | | | | | 1.00 25.42 |
| ATOM | 2978 | CG | ARG | 429 | -4.594 | 22.731 | 34.106 | |
| MOTA | 2979 | CD | ARG | 429 | -4.832 | 21.643 | 33.064 | 1.00 21.31 |
| MOTA | 2980 | NE | ARG | 429 | -6.072 | 20.932 | 33.372 | 1.00 20.15 |
| MOTA | 2981 | CZ | ARG | 429 | -7.270 | 21.513 | 33.413 | 1.00 19.59 |
| ATOM | 2982 | NH1 | ARG | 429 | -7.396 | 22.805 | 33.157 | 1.00 19.16 |
| ATOM | 2983 | NH2 | ARG | 429 | -8.340 | 20.815 | 33.736 | 1.00 18.53 |
| MOTA | 2984 | С | ARG | 429 | -1.930 | 25.423 | 34.825 | 1.00 28.16 |
| ATOM | 2985 | 0 | ARG | 429 | -0.934 | 24.708 | 34.728 | 1.00 27.12 |
| ATOM | 2986 | N | ALA | 430 | -1.865 | 26.742 | 34.990 | 1.00 29.24 |
| ATOM | 2987 | CA | ALA | 430 | -0.600 | 27.464 | 35.109 | 1.00 29.49 |
| MOTA | 2988 | CB | ALA | 430 | 0.233 | 26.864 | 36.237 | 1.00 29.80 |
| ATOM | 2989 | C | ALA | 430 | 0.239 | 27.544 | 33.834 | 1.00 29.79 |
| ATOM | 2990 | Ö | ALA | 430 | 1.468 | 27.521 | 33.900 | 1.00 30.37 |
| ATOM | 2991 | N | VAL | 431 | -0.409 | 27.641 | 32.676 | 1.00 29.07 |
| ATOM | 2992 | CA | VAL | 431 | 0.332 | 27.738 | 31.420 | 1.00 27.53 |
| ATOM | 2993 | CB | VAL | 431 | 0.279 | 26.405 | 30.623 | 1.00 27.98 |
| | 2994 | | | 431 | 1.073 | 26.545 | 29.327 | 1.00 27.35 |
| ATOM | | | VAL | | | | | |
| ATOM | 2995 | | VAL | 431 | 0.848 | 25.274 | 31.457 | 1.00 25.30 |
| MOTA | 2996 | C | VAL | 431 | -0.175 | 28.866 | 30.522 | 1.00 27.45 |
| ATOM | 2997 | 0 | VAL | 431 | -1.231 | 28.750 | 29.894 | 1.00 27.25 |
| MOTA | 2998 | N | PRO | 432 | 0.570 | 29.986 | 30.460 | 1.00 26.79 |
| MOTA | 2999 | CD | PRO | 432 | 1.831 | 30.287 | 31.155 | 1.00 26.11 |
| ATOM | 3000 | CA | PRO | 432 | 0.159 | 31.115 | 29.617 | 1.00 26.19 |
| ATOM . | 3001 | CB | PRO | 432 | 1.135 | 32.218 | 30.017 | 1.00 27.09 |
| ATOM | 3002 | CG | PRO | 432 | 2.360 | 31.452 | 30.362 | 1.00 29.57 |
| ATOM | 3003 | С | PRO | 432 | 0.285 | 30.715 | 28.152 | 1.00 24.89 |
| MOTA | 3004 | 0 | PRO | 432 | 1.205 | 29.987 | 27.775 | 1.00 24.44 |
| ATOM | 3005 | N | VAL | 433 | -0.642 | 31.192 | 27.333 | 1.00 23.55 |
| ATOM | 3006 | CA | VAL | 433 | -0.653 | | 25.924 | 1.00 22.49 |
| ATOM | 3007 | CB | VAL | 433 | -1.895 | 29.990 | 25.592 | 1.00 20.80 |
| ATOM | 3008 | | VAL | 433 | -1.915 | 29.640 | 24.111 | 1.00 21.86 |
| ATOM | 3009 | CG2 | VAL | 433 | -1.896 | 28.726 | 26.449 | 1.00 19.73 |
| ATOM | 3010 | C | VAL | 433 | -0.633 | 32.030 | 24.980 | 1.00 24.12 |
| ATOM | 3011 | 0 | VAL | 433 | -1.244 | 33.068 | 25.244 | 1.00 22.28 |
| | 3012 | N | CYS | 434 | 0.091 | 31.850 | 23.880 | 1.00 25.46 |
| ATOM | | | | | 0.206 | | 22.820 | 1.00 26.20 |
| ATOM | 3013 | CA | CYS | 434 | | 32.841 | | |
| MOTA | 3014 | CB | CYS | 434 | 1.675 | 33.159 | 22.543 | 1.00 27.30 |
| ATOM | 3015 | SG | CYS | 434 | 1.936 | 34.229 | 21.110 | 1.00 29.19 |
| ATOM | 3016 | C | CYS | 434 | -0.416 | 32.197 | 21.585 | 1.00 27.10 |
| ATOM | 3017 | 0 | CYS | 434 | 0.010 | 31.123 | 21.165 | 1.00 27.48 |
| MOTA | 3018 | N | GLY | 435 | -1.428 | 32.842 | 21.019 | 1.00 25.59 |
| MOTA | 3019 | CA | GLY | 435 | -2.078 | 32.298 | 19.842 | 1.00 27.29 |
| MOTA | 3020 | С | GLY | 435 | -1.269 | 32.541 | 18.586 | 1.00 27.32 |
| MOTA | 3021 | 0 | GLY | 435 | -0.237 | 33.211 | 18.629 | 1.00 26.82 |
| MOTA | 3022 | N | HIS | 436 | -1.737 | 32.005 | 17.463 | 1.00 27.79 |
| MOTA | 3023 | CA | HIS | 436 | -1.037 | 32.164 | 16.195 | 1.00 28.13 |
| MOTA | 3024 | СВ | HIS | 436 | 0.117 | 31.158 | 16.128 | 1.00 28.29 |
| MOTA | 3025 | CG | HIS | 436 | 1.044 | 31.362 | 14.970 | 1.00 29.67 |
| ATOM | 3026 | | HIS | 436 | 0.893 | 32.043 | 13.809 | 1.00 28.18 |
| ATOM | 3027 | | HIS | 436 | 2.298 | 30.792 | 14.918 | 1.00 28.22 |
| ATOM | 3028 | | HIS | 436 | 2.878 | 31.110 | 13.775 | 1.00 29.12 |
| ATOM | 3029 | | HIS | 436 | 2.046 | 31.868 | 13.083 | 1.00 27.13 |
| ATOM | 3030 | C | HIS | 436 | -2.008 | 31.950 | 15.039 | 1.00 29.59 |
| | 3031 | 0 | HIS | 436 | -2.356 | 30.817 | 14.708 | 1.00 27.47 |
| MOTA | | | | せつひ | 2.220 | JU.UI/ | , 00 | |

| ATOM | 3032 | N | LEU | 437 | -2.442 | 33.052 | 14.428 | 1.00 30.59 |
|--------|-------|------|------|-------|--------|--------|--------|------------|
| | | | | | -3.384 | 32.999 | 13.314 | 1.00 31.59 |
| ATOM | 3033 | CA | LEU | 437 | | | | |
| ATOM | 3034 | CB | LEU | 437 | -4.632 | 33.823 | 13.643 | 1.00 31.44 |
| ATOM | 3035 | CG | LEU | 437 | -5.519 | 33.332 | 14.790 | 1.00 30.60 |
| | | | LEU | 437 | -6.611 | 34.351 | 15.065 | 1.00 30.46 |
| ATOM | 3036 | | | | | | | |
| ATOM | 3037 | CD2 | LEU | 437 | -6.124 | 31.978 | 14.429 | 1.00 30.85 |
| MOTA | 3038 | С | LEU | 437 | -2.771 | 33.507 | 12.015 | 1.00 32.51 |
| ATOM | 3039 | 0 | LEU | 437 | -1.758 | 34.204 | 12.024 | 1.00 32.44 |
| | | | | | | | | |
| ATOM | 3040 | N | GLY | 438 | -3.399 | 33.154 | 10.898 | 1.00 34.06 |
| ATOM | 3041 | CA | GLY | 438 | ~2.905 | 33.587 | 9.606 | 1.00 35.62 |
| ATOM | 3042 | С | GLY | 438 | -2.283 | 32.452 | 8.825 | 1.00 37.37 |
| | | | | 438 | -2.896 | 31.400 | 8.641 | 1.00 37.17 |
| ATOM | 3043 | 0 | GLY | | | | | |
| MOTA | 3044 | N | LEU | 439 | -1.055 | 32.659 | 8.366 | 1.00 38.61 |
| ATOM | 3045 | CA | LEU | 439 | -0.355 | 31.642 | 7.601 | 1.00 39.93 |
| | 3046 | CB | LEU | 439 | 0.623 | 32.310 | 6.630 | 1.00 42.55 |
| MOTA | | | | | | | | |
| ATOM | 3047 | CG | LEU | 439 | 1.104 | 31.510 | 5.414 | 1.00 44.13 |
| ATOM | 3048 | CD1 | LEU | 439 | 1.964 | 32.410 | 4.533 | 1.00 45.83 |
| ATOM | 3049 | CD2 | LEU | 439 | 1.889 | 30.288 | 5.858 | 1.00 43.74 |
| | | | | | 0.388 | 30.719 | 8.567 | 1.00 40.30 |
| ATOM | 3050 | С | LEU | 439 | | | | |
| ATOM | 3051 | 0 | LEU | 439 | 1.549 | 30.957 | 8.902 | 1.00 40.50 |
| ATOM | 3052 | N | THR | 440 | -0.302 | 29.675 | 9.020 | 1.00 39.46 |
| ATOM | 3053 | CA | THR | 440 | 0.267 | 28.700 | 9.947 | 1.00 38.93 |
| | | | | | | | | |
| ATOM | 3054 | CB | THR | 440 | -0.847 | 27.967 | 10.717 | 1.00 39.18 |
| ATOM | 3055 | OG1 | THR | 440 | -1.763 | 27.374 | 9.787 | 1.00 38.96 |
| MOTA | 3056 | CG2 | THR | 440 | -1.600 | 28.938 | 11.612 | 1.00 37.57 |
| | | | | 440 | 1.108 | 27.677 | 9.181 | 1.00 38.59 |
| ATOM | 3057 | С | THR | | | | | |
| MOTA | 3058 | 0 | THR | 440 | 0.572 | 26.785 | 8.522 | 1.00 38.96 |
| MOTA | 3059 | N | PRO | 441 | 2.444 | 27.791 | 9.270 | 1.00 37.45 |
| ATOM | 3060 | CD | PRO | 441 | 3.166 | 28.736 | 10.142 | 1.00 37.29 |
| | | | | | | | | |
| ATOM | .3061 | CA | PRO | 441 | 3.378 | 26.891 | 8.586 | 1.00 36.21 |
| ATOM | 3062 | CB | PRO | 441 | 4.747 | 27.433 | 8.998 | 1.00 36.37 |
| ATOM | 3063 | CG . | PRO | 441 | 4.485 | 28.045 | 10.332 | 1.00 39.17 |
| | | | | 441 | 3.205 | 25.400 | 8.882 | 1.00 34.87 |
| MOTA | 3064 | C | PRO | | | | | |
| MOTA | 3065 | 0 | PRO | 441 | 3.548 | 24.558 | 8.050 | 1.00 33.70 |
| MOTA | 3066 | N | GLN | 442 | 2.677 | 25.069 | 10.058 | 1.00 33.93 |
| ATOM | 3067 | CA | GLN | 442 | 2.453 | 23.668 | 10.406 | 1.00 32.20 |
| | | | | | | | | 1.00 31.74 |
| ATOM | 3068 | CB | GLN | 442 | 1.991 | 23.542 | 11.863 | |
| ATOM | 3069 | CG | GLN | 442 | 3.122 | 23.343 | 12.873 | 1.00 29.51 |
| ATOM | 3070 | CD | GLN | 442 | 2.644 | 23.472 | 14.312 | 1.00 29.21 |
| | | | | 442 | 1.579 | 22.972 | 14.670 | 1.00 27.25 |
| MOTA | 3071 | | GLN | | | | | |
| MOTA | 3072 | NE2 | GLN | 442 | 3.436 | 24.136 | 15.145 | 1.00 28.44 |
| ATOM | 3073 | С | GLN | 442 | 1.406 | 23.052 | 9.472 | 1.00 31.45 |
| MOTA | 3074 | 0 | GLN | 442 | 1.423 | 21.848 | 9.215 | 1.00 30.71 |
| | | | | | | | | |
| MOTA | 3075 | N | SER | 443 | 0.500 | 23.885 | 8.965 | 1.00 30.60 |
| ATOM | 3076 | CA | SER | 443 | -0.546 | 23.420 | 8.058 | 1.00 31.30 |
| ATOM | 3077 | CB | SER | 443 | -1.881 | 24.089 | 8.394 | 1.00 31.62 |
| | 3078 | OG | SER | 443 | -2.343 | 23.707 | | 1.00 32.96 |
| ATOM | | | | | | | | |
| MOTA | 3079 | С | SER | 443 | -0.188 | 23.711 | 6.603 | 1.00 30.60 |
| ATOM | 3080 | 0 | SER | 443 | -1.070 | 23.829 | 5.751 | 1.00 29.98 |
| ATOM | 3081 | N | VAL | 444 | 1.109 | 23.818 | 6.323 | 1.00 29.83 |
| | | | | 444 | | | | |
| MOTA | 3082 | CA | VAL | | 1.590 | 24.101 | 4.970 | 1.00 29.28 |
| MOTA | 3083 | CB | VAL | 444 | 3.143 | 24.079 | 4.909 | 1.00 30.47 |
| ATOM | 3084 | CG1 | VAL | 444 | 3.670 | 22.706 | 5.307 | 1.00 28.85 |
| ATOM | 3085 | | VAL | 444 | 3.616 | 24.440 | 3.504 | 1.00 30.63 |
| | | | | | | | | |
| MOTA | 3086 | С | VAL | 444 | 1.039 | 23.101 | 3.952 | |
| MOTA | 3087 | 0 | VAL | 444 | 0.718 | 23.466 | 2.819 | 1.00 30.16 |
| ATOM | 3088 | N | ASN | 445. | 0.925 | 21.842 | 4.361 | 1.00 28.62 |
| ATOM | 3089 | CA | ASN | 445 | 0.412 | 20.804 | 3.478 | 1.00 27.90 |
| | | | | | | | | 1.00 26.96 |
| MOTA | 3090 | CB | ASN | 445 | 0.666 | 19.425 | 4.089 | |
| ATOM | 3091 | CG | ASN | 445 | 2.141 | 19.128 | 4.245 | 1.00 28.30 |
| ATOM | 3092 | OD1 | ASN | 445 | 2.868 | 19.009 | 3.257 | 1.00 30.31 |
| | 3093 | | ASN | 445 | 2.598 | 19.023 | 5.488 | 1.00 28.01 |
| MOTA | | | | | | | | |
| MOTA | 3094 | C | ASN | 445 | -1.073 | 20.991 | 3.203 | 1.00 27.73 |
| ATOM | 3095 | 0 | ASN | 445 | -1.575 | 20.566 | 2.165 | 1.00 25.69 |
| ATOM | 3096 | N | ILE | 446 | -1.767 | 21.632 | 4.138 | 1.00 29.28 |
| | | | | | -3.196 | 21.890 | 3.993 | 1.00 31.96 |
| ATOM | 3097 | CA | ILE | 446 | | | | |
| ATOM | 3098 | CB | ILE | 446 | ~3.836 | 22.319 | 5.335 | 1.00 31.98 |
| MOTA | 3099 | CG2 | ILE | 446 | ~5.264 | 22.799 | 5.105 | 1.00 31.16 |
| ATOM | 3100 | CG1 | ILE | 446 | -3.814 | 21.153 | 6.331 | 1.00 30.13 |
| | | | | | | | | |
| ATOM | 3101 | | ILE | 446 | -4.670 | 19.979 | 5.928 | 1.00 31.79 |
| MOTA | 3102 | С | ILE | 446 | -3.411 | 23.007 | 2.982 | 1.00 34.41 |
| ATOM | 3103 | 0 | ILE | 446 | -4.239 | 22.889 | 2.080 | 1.00 33.82 |
| ATOM | 3104 | N | PHE | 447 | -2.657 | 24.092 | 3.142 | 1.00 36.64 |
| | | | | | | | | |
| ATOM | 3105 | CA | PHE | 447 | -2.763 | 25.245 | 2.249 | 1.00 39.97 |
| ATOM | 3106 | CB | PHE | 447 | -2.040 | 26.452 | 2.852 | 1.00 39.70 |
| ATOM | 3107 | CG | PHE | 447 . | -2.516 | 26.826 | 4.228 | 1.00 40.98 |
| ATOM | 3108 | | PHE | 447 | -3.860 | 27.100 | 4.467 | 1.00 41.63 |
| 111/11 | 2100 | CDI | EIIE | / | 5.000 | 27.100 | 4.407 | 41.03 |
| | | | | | | | | |

| MOTA | 3109 | CD2 | PHE | 447 | -1.613 | 26.931 | 5.282 | 1.00 41.49 |
|------|------|-----|-----|------------|---------|--------|--------|------------|
| ATOM | 3110 | | PHE | 447 | -4.299 | 27.474 | 5.738 | 1.00 41.71 |
| ATOM | 3111 | CE2 | PHE | 447 | -2.040 | 27.304 | 6.557 | 1.00 41.93 |
| ATOM | 3112 | CZ | PHE | 447 | -3.388 | 27.577 | 6.785 | 1.00 41.96 |
| | 3113 | C | PHE | 447 | -2.170 | 24.948 | 0.874 | 1.00 42.08 |
| ATOM | | | PHE | 447 | -2.536 | 25.579 | -0.121 | 1.00 42.68 |
| MOTA | 3114 | 0 | | | -1.251 | 23.987 | 0.831 | 1.00 42.00 |
| MOTA | 3115 | N | GLY | 448 | | | | 1.00 45.71 |
| MOTA | 3116 | CA | GLY | 448 | -0.608 | 23.622 | -0.418 | |
| MOTA | 3117 | С | GLY | 448 | 0.576 | 24.528 | -0.695 | 1.00 47.94 |
| ATOM | 3118 | 0 | GLY | 448 | 0.963 | 24.729 | -1.846 | 1.00 48.22 |
| MOTA | 3119 | N | GLY | 449 | 1.150 | 25.076 | 0.371 | 1.00 49.19 |
| MOTA | 3120 | CA | GLY | 449 | 2.285 | 25.969 | 0.239 | 1.00 50.57 |
| MOTA | 3121 | С | GLY | 449 | 2.149 | 27.142 | 1.191 | 1.00 51.89 |
| MOTA | 3122 | 0 | GLY | 449 | 1.263 | 27.148 | 2.047 | 1.00 51.79 |
| MOTA | 3123 | N | TYR | 450 | 3.020 | 28.137 | 1.048 | 1.00 53.06 |
| MOTA | 3124 | CA | TYR | 450 | 2.970 | 29.311 | 1.912 | 1.00 54.66 |
| MOTA | 3125 | CB | TYR | 450 | 4.375 | 29.674 | 2.397 | 1.00 54.86 |
| ATOM | 3126 | CG | TYR | 450 | 5.085 | 28.537 | 3.093 | 1.00 55.77 |
| MOTA | 3127 | | TYR | 450 | 5.758 | 27.559 | 2.362 | 1.00 55.77 |
| ATOM | 3128 | | TYR | 450 | 6.387 | 26.490 | 2.996 | 1.00 56.62 |
| ATOM | 3129 | | TYR | 450 | 5.057 | 28.420 | 4.482 | 1.00 55.92 |
| ATOM | 3130 | CE2 | TYR | 450 | 5.681 | 27.354 | 5.128 | 1.00 56.38 |
| ATOM | 3131 | CZ | TYR | 450 | 6.344 | 26.392 | 4.378 | 1.00 56.70 |
| ATOM | 3132 | OH | TYR | 450 | 6.958 | 25.329 | 5.008 | 1.00 56.18 |
| | 3133 | C | TYR | 450 | 2.346 | 30.493 | 1.178 | 1.00 55.36 |
| MOTA | | | | | 3.036 | 31.265 | 0.513 | 1.00 55.48 |
| ATOM | 3134 | 0 | TYR | 450 | | | | |
| ATOM | 3135 | N | LYS | 451 | 1.031 | 30.625 | 1.311 | 1.00 56.14 |
| ATOM | 3136 | CA | LYS | 451 | 0.291 | 31.695 | 0.659 | 1.00 56.56 |
| ATOM | 3137 | CB | LYS | 451 | -0.833 | 31.099 | -0.189 | 1.00 57.29 |
| ATOM | 3138 | CG | LYS | 451 | -0.410 | 29.887 | -1.008 | 1.00 57.70 |
| ATOM | 3139 | CD | LYS | 451 | -1.613 | 29.188 | -1.621 | 1.00 58.82 |
| MOTA | 3140 | CE | LYS | 451 | -1.232 | 27.840 | -2.215 | 1.00 58.93 |
| MOTA | 3141 | NZ | LYS | 451 | -2.426 | 27.115 | -2.731 | 1.00 58.99 |
| MOTA | 3142 | С | LYS | 451 | -0.296 | 32.626 | 1.714 | 1.00 56.60 |
| ATOM | 3143 | 0 | LYS | 451 | -0.542 | 32.216 | 2.849 | 1.00 56.17 |
| ATOM | 3144 | N | VAL | 452 | -0.521 | 33.879 | 1.333 | 1.00 56.36 |
| ATOM | 3145 | CA | VAL | 452 | -1.079 | 34.868 | 2.245 | 1.00 56.35 |
| MOTA | 3146 | CB | VAL | 452 | -0.945 | 36.297 | 1.667 | 1.00 56.62 |
| ATOM | 3147 | CG1 | VAL | 452 | -1.394 | 37.322 | 2.696 | 1.00 56.98 |
| ATOM | 3148 | | VAL | 452 | 0.491 | 36.553 | 1.247 | 1.00 56.04 |
| ATOM | 3149 | C | VAL | 452 | -2.557 | 34.591 | 2.514 | 1.00 56.29 |
| ATOM | 3150 | 0 | VAL | 452 | -3.383 | 34.631 | 1.600 | 1.00 56.01 |
| ATOM | 3151 | N | GLN | 453 | -2.880 | 34.304 | 3.772 | 1.00 56.06 |
| ATOM | 3152 | CA | GLN | 453 | -4.258 | 34.036 | 4.166 | 1.00 56.41 |
| ATOM | 3153 | CB | GLN | 453 | -4.303 | 33.044 | 5.334 | 1.00 56.31 |
| ATOM | 3154 | CG | GLN | 453 | -4.304 | 31.574 | 4.926 | 1.00 56.61 |
| ATOM | 3155 | CD | GLN | 453 | -3.011 | 31.138 | 4.268 | 1.00 57.19 |
| | | | | 453 | -1.934 | 31.255 | 4.854 | 1.00 57.65 |
| ATOM | 3156 | | GLN | | -3.111 | 30.624 | 3.048 | 1.00 55.74 |
| ATOM | 3157 | NE2 | GLN | 453 | | | 4.565 | |
| ATOM | 3158 | C | GLN | 453 | -4.965 | 35.327 | | 1.00:56.38 |
| ATOM | 3159 | 0 | GLN | 453 | -4.333 | 36.375 | 4.704 | 1.00 55.54 |
| ATOM | 3160 | N | GLY | 454 | -6.281 | 35.244 | 4.746 | 1.00 56.76 |
| ATOM | 3161 | CA | GLY | 454 | -7.053 | 36.413 | 5.127 | 1.00 57.88 |
| ATOM | 3162 | С | GLY | 454 | -7.627 | 37.165 | 3.940 | 1.00 58.46 |
| ATOM | 3163 | 0 | GLY | 454 | -8.382 | 38.120 | 4.115 | 1.00 58.43 |
| ATOM | 3164 | N | ARG | 455 | -7.267 | 36.735 | 2.733 | 1.00 59.53 |
| ATOM | 3165 | CA | ARG | 455 | -7.750 | 37.371 | 1.509 | 1.00 61.02 |
| MOTA | 3166 | CB | ARG | 455 | -7.081 | 36.737 | 0.283 | 1.00 61.22 |
| MOTA | 3167 | CG | ARG | 455 | -5.603 | 37.080 | 0.120 | 1.00 61.34 |
| ATOM | 3168 | CD | ARG | 455 | -5.416 | 38.532 | -0.305 | 1.00 61.58 |
| MOTA | 3169 | NE | ARG | 455 | -4.023 | 38.979 | -0.232 | 1.00 61.55 |
| MOTA | 3170 | CZ | ARG | 455 | -3.013 | 38.444 | -0.914 | 1.00 60.83 |
| MOTA | 3171 | NH1 | ARG | 455 | -3.224 | 37.425 | -1.736 | 1.00 60.33 |
| MOTA | 3172 | NH2 | ARG | 455 | -1.788 | 38.935 | -0.778 | 1.00 60.86 |
| ATOM | 3173 | С | ARG | 455 | -9.268 | 37.252 | 1.387 | 1.00 61.98 |
| ATOM | 3174 | 0 | ARG | 455 | -9.805 | 36.157 | 1.214 | 1.00 61.66 |
| ATOM | 3175 | N | GLY | 456 | -9.955 | 38.387 | 1.482 | 1.00 62.93 |
| АТОМ | 3176 | CA | GLY | 456 | -11.402 | 38.386 | 1.379 | 1.00 64.13 |
| ATOM | 3177 | C | GLY | 456 | -12.084 | 38.769 | 2.678 | 1.00 65.08 |
| ATOM | 3178 | ō | GLY | 456 | -11.445 | 38.843 | 3.728 | 1.00 65.12 |
| ATOM | 3179 | N | ASP | 457 | -13.388 | 39.016 | 2.606 | 1.00 65.45 |
| ATOM | 3180 | CA | ASP | 457 | -14.162 | 39.392 | 3.783 | 1.00 65.79 |
| ATOM | 3181 | CB | ASP | 457 | -15.457 | 40.094 | 3.765 | 1.00 66.87 |
| ATOM | 3182 | CG | ASP | 457 | -15.205 | 41.358 | 2.565 | 1.00 67.41 |
| | | | | | -14.544 | | 3.095 | 1.00 67.41 |
| ATOM | 3183 | | ASP | 457 457 | | 42.277 | | |
| ATOM | 3184 | | ASP | 457 | -15.668 | 41.432 | 1.407 | 1.00 68.24 |
| MOTA | 3185 | С | ASP | 457 | -14.494 | 38.159 | 4.616 | 1.00 65.50 |

| ATOM | 3186 | 0 | ASP | 457 | -14.485 | 38.208 | 5.846 | 1.00 65.44 |
|--------------|--------------|-----|------------|------------|--------------------|------------------|------------------|--------------------------|
| ATOM | 3187 | N | GLU | 458 | -14.788 | 37.055 | 3.936 | 1.00 65.17 |
| ATOM | 3188 | CA | GLU | 458 | -15.122 | 35.808 | 4.611 | 1.00 64.76 |
| ATOM | 3189 | CB | GLU | 458 | -15.460 | 34.726 | 3.583 | 1.00 65.72 |
| ATOM | 3190 | CG | GLU | 458 | -15.856 | 33.392 | 4.194 | 1.00 67.79 |
| ATOM | 3191 | CD | GLU | 458 | -16.235 | 32.360 | 3.149 | 1.00 68.91 |
| ATOM | 3192 | OE1 | | 458 | -17.201 | 32.605 | 2.394 | 1.00 69.70 |
| АТОМ | 3193 | | GLU | 458 | -15.568 | 31.305 | 3.083 | 1.00 69.17 |
| ATOM | 3194 | С | GLU | 458 | -13.956 | 35.348 | 5.480 | 1.00 63.98 |
| ATOM | 3195 | 0 | GLU | 458 | -14.115 | 35.121 | 6.681 | 1.00 63.71 |
| ATOM | 3196 | N | ALA | 459 | -12.785 | 35.213 | 4.866 | 1.00 62.74 |
| ATOM | 3197 | CA | ALA | 459 | -11.588 | 34.787 | 5.581 | 1.00 61.25 |
| ATOM | 3198 | CB | ALA | 459 | -10.462 | 34.507 | 4.594 | 1.00 61.27 |
| ATOM | 3199 | C | ALA | 459 | -11.159 | 35.863 | 6.575 | 1.00 60.06 |
| MOTA | 3200 | 0 | ALA | 459 | -10.630 | 35.560 | 7.645 | 1.00 59.75 |
| ATOM | 3201 | N | GLY | 460 | -11.392 | 37.119 | 6.212 | 1.00 58.46 |
| MOTA | 3202 | CA | GLY | 460 | -11.029 | 38.218 | 7.083 | 1.00 57.13 |
| ATOM | 3203 | С | GLY | 460 | -11.808 | 38.207 | 8.384 | 1.00 56.78 |
| MOTA | 3204 | 0 | GLY | 460 | -11.220 | 38.275 | 9.463 | 1.00 56.93 |
| MOTA | 3205 | N | ASP | 461 | -13.132 | 38.118 | 8.290 | 1.00 55.32 |
| ATOM | 3206 | CA | ASP | 461 | -13.974 | 38.101 | 9.481 | 1.00 54.77 |
| ATOM | 3207 | CB | ASP | 461 | -15.455 | 38.211 | 9.099 | 1.00 55.32 |
| MOTA | 3208 | CG | ASP | 461 | -15.783 | 39.512 | 8.386 | 1.00 56.16 |
| MOTA | 3209 | OD1 | ASP | 461 | -15.440 | 40.593 | 8.913 | 1.00 56.40 |
| ATOM | 3210 | OD2 | ASP | 461 | -16.395 | 39.452 | 7.301 | 1.00 56.69 |
| MOTA | 3211 | С | ASP | 461 | -13.753 | 36.825 | 10.287 | 1.00 53.74 |
| MOTA | 3212 | Ο. | ASP | 461 | -13.998 | 36.792 | 11.491 | 1.00 53.31 |
| MOTA | 3213 | N | GLN | 462 | -13.290 | 35.776 | 9.614 | 1.00 53.09 |
| ATOM | 3214 | CA | GLN | 462 | -13.034 | 34.500 | 10.268 | 1.00 52.15 |
| MOTA | 3215 | CB | GLN | 462 | -12.908 | 33.387 | 9.228 | 1.00 51.74 |
| ATOM | 3216 | CG | GLN | 462 | -12.684 | 32.009 | 9.826 | 1.00 51.57 |
| MOTA | 3217 | CD | GLN | 462 | -13.729 | 31.655 | 10.865 | 1.00 52.18 |
| MOTA | 3218 | OE1 | GLN | .462 | -14.930 | 31.725 | 10.604 | 1.00 51.90 |
| MOTA | 3219 | | GLN | 462 | -13.275 | 31.268 | 12.053 | 1.00 52.39 |
| MOTA | 3220 | С | GLN | 462 | -11.767 | 34.567 | 11.108 | 1.00 51.68 |
| ATOM | 3221 | 0 | GLN | 462 | -11.647 | 33.878 | 12.121 | 1.00 52.10 |
| MOTA | 3222 | N | LEU | 463 | -10.819 | 35.397 | 10.686 | 1.00 51.14 |
| ATOM | 3223 | CA | LEU | 463 | -9.567 | 35.552 | 11.419 | 1.00 50.31 |
| ATOM | 3224 | CB | LEU | 463 | -8.478 | 36.116 | 10.507 | 1.00 51.43 |
| ATOM | 3225 | CG | LEU | 463 | -8.036 | 35.227 | 9.343 | 1.00 52.52 |
| ATOM | 3226 | | LEU | 463 | -6.962 | 35.949 | 8.542 | 1.00 53.49 |
| MOTA | 3227 | | LEU | 463 | -7.505 | 33.901 | 9.872 | 1.00 53.21 |
| ATOM | 3228 | C | LEU | 463 | -9.769 | 36.480 | 12.603 | 1.00 49.29 |
| MOTA | 3229 | 0 | LEU | 463 | -9.162 | 36.295 | 13.656 | 1.00 49.00 |
| MOTA | 3230 | N | LEU | 464 | -10.622 | 37.483 | 12.424 | 1.00 48.83 |
| ATOM | 3231 | CA | LEU | 464 | -10.907 | 38.439 | 13.488 | 1.00 48.51 |
| MOTA | 3232 | CB | LEU | 464 | -11.724 | 39.613 | 12.939 | 1.00 48.82 |
| ATOM | 3233 | CG. | LEU | 464 | -11.609 | 40.957 | 13.668 | 1.00 50.56 1.00 50.81 |
| ATOM | 3234 | | LEU | 464 | -12.492 -12.017 | 41.976 | 12.960 15.126 | 1.00 50.81 |
| ATOM | 3235 3236 | CD2 | LEU | 464 464 | -11.697 | 40.827 37.725 | 14.582 | 1.00 46.83 |
| MOTA | 3237 | 0 | LEU | 464 | -11.657 | 37.723 | 15.772 | 1.00 46.51 |
| ATOM ATOM | 3237 | N | | 465 | -12.626 | 36.867 | 14.165 | 1.00 45.83 |
| ATOM | 3239 | CA | SER SER | 465 | -13.452 | 36.104 | 15.095 | 1.00 43.65 |
| ATOM | 3240 | CB | SER | 465 | -14.506 | 35.295 | 14.335 | 1.00 45.80 |
| ATOM | 3241 | OG | SER | 465 | -15.284 | 34.505 | 15.225 | 1.00 45.26 |
| ATOM | 3242 | C | SER | 465 | -12.576 | 35.156 | 15.900 | 1.00 43.62 |
| ATOM | 3243 | ō | SER | 465 | -12.702 | 35.072 | 17.119 | 1.00 43.30 |
| ATOM | 3244 | N | ASP | 466 | -11.700 | 34.435 | 15.205 | 1.00 41.72 |
| ATOM | 3245 | CA | ASP | 466 | -10.796 | 33.503 | 15.867 | 1.00 40.59 |
| ATOM | 3246 | СВ | ASP | 466 | -9.941 | 32.742 | 14.847 | 1.00 40.56 |
| ATOM | 3247 | CG | ASP | 466 | -10.730 | | 14.086 | 1.00 41.88 |
| ATOM | 3248 | | ASP | 466 | -11.651 | 31.083 | 14.674 | 1.00 43.44 |
| MOTA | 3249 | | ASP | 466 | -10.418 | 31.458 | 12.902 | 1.00 41.17 |
| ATOM | 3250 | С | ASP | 466 | -9.885 | 34.265 | 16.817 | 1.00 38.59 |
| ATOM | 3251 | Ō | ASP | 466 | -9.566 | 33.780 | 17.900 | 1.00 37.69 |
| MOTA | 3252 | N | ALA | 467 | -9.472 | 35.460° | 16,408 | 1.00 37.24 |
| ATOM | 3253 | CA | ALA | 467 | -8.596 | 36.291 - | 17.226 | 1.00 36.59 |
| MOTA | 3254 | СВ | ALA | 467 | -8.232 | 37.568 | 16.472 | 1.00 35.34 |
| MOTA | 3255 | С | ALA | 467 | -9.284 | 36.635 | 18.541 | 1.00 36.59 |
| MOTA | 3256 | 0 | ALA | 467 | -8.707 | 36.477 | 19.616 | 1.00 36.56 |
| MOTA | 3257 | N | LEU | 468 | -10.520 | 37.116 | 18.450 | 1.00 36.29 |
| MOTA | 3258 | CA | LEU | 468 | -11.283 | 37.465 | 19.643 | 1.00 36.13 |
| MOTA | 3259 | CB | LEU | 468 | -12.610 | 38.119 | 19.254 | 1.00 36.56 |
| MOTA | 3260 | CG | LEU | 468 | -12.551 | 39.555 | 18.732 | 1.00 38.68 |
| MOTA | 3261 | | LEU | 468 | -13.871 | 39.910 | 18.062 | 1.00 40.41 |
| MOTA | 3262 | CD2 | LEU | 468 | -12.248 | 40.501 | 19.884 | 1.00 38.41 |

| ATOM | 3263 | С | LEU | 468 | -11.559 | 36.204 | 20.452 | 1.00 35.67 |
|--------------|--------------|-----------|------------|------------|-------------------|------------------|------------------|--------------------------|
| ATOM | 3264 | 0 | LEU | 468 | -11.565 | 36.232 | 21.683 | 1.00 36.76 |
| MOTA | 3265 | N | ALA | 469 | -11.788 | 35.099 | 19.747 | 1.00 34.59 |
| ATOM | 3266 | CA | ALA | 469 | -12.077 | 33.820 | 20.387 | 1.00 34.17 |
| MOTA | 3267 | СВ | ALA | 469 | | 32.768 | 19.332 | 1.00 33.45 |
| MOTA | 3268 | С | ALA | 469 | -10.917 | 33.370 | 21.269 | 1.00 34.41 |
| ATOM. | 3269 | 0 | ALA | 469 | -11.101 | 33.073 | 22.453 | 1.00 33.82 |
| ATOM | 3270 | N | LEU | 470 | -9.725 | 33.315 | 20.685 | 1.00 33.79 |
| ATOM | 3271 3272 | CA | LEU LEU | 470 470 | -8.534 -7.297 | 32.911 32.981 | 21.420 20.516 | 1.00 34.13 1.00 33.55 |
| ATOM ATOM | 3272 | CB CG | LEU | 470 | -7.261 | 32.931 | 19.317 | 1.00 33.55 |
| ATOM. | 3274 | CD1 | | 470 | -6.006 | 32.282 | 18.490 | 1.00 32.93 |
| ATOM | 3275 | CD2 | | 470 | -7.289 | 30.589 | 19.803 | 1.00 32.13 |
| MOTA | 3276 | С | LEU | 470 | -8.347 | 33.816 | 22.627 | 1.00 34.20 |
| MOTA | 3277 | 0 | LEU | 470 | -8.061 | 33.347 | 23.732 | 1.00 34.77 |
| MOTA | 3278 | N | GLU | 471 | -8.516 | 35.119 | 22.417 | 1.00 33.48 |
| MOTA | 3279 | CA | GLU | 471 | -8.373 | 36.085 | 23.499 | 1.00 33.79 |
| ATOM | 3280 | CB | GLU | 471 | -8.594 | 37.506 | 22.978 | 1.00 34.37 |
| MOTA | 3281 | CG | GLU | 471 | -8.617 | 38.553 | 24.080 | 1.00 35.68 |
| MOTA | 3282 3283 | CD OE1 | GLU | 471 471 | -8.985 -10.028 | 39.930 40.055 | 23.565 22.881 | 1.00 36.13 1.00 36.43 |
| ATOM ATOM | 3284 | | GLU | 471 | -8.233 | 40.884 | 23.851 | 1.00 35.43 |
| MOTA | 3285 | C | GLU | 471 | -9.376 | 35.796 | 24.613 | 1.00 33.42 |
| ATOM | 3286 | 0 | GLU | 471 | -9.022 | 35.778 | 25.793 | 1.00 32.79 |
| MOTA | 3287 | N | ALA | 472 | -10.631 | 35.584 | 24.232 | 1.00 33.45 |
| MOTA | 3288 | CA | ALA | 472 | -11.672 | 35.291 | 25.209 | 1.00 32.67 |
| MOTA | 3289 | CB | ALA | 472 | -13.019 | 35.130 | 24.506 | 1.00 32.92 |
| MOTA | 3290 | C | ALA | | -11.308 | 34.015 | 25.963 | 1.00 32.35 |
| ATOM | 3291 | 0 | ALA | 472 | -11.559 | 33.900 | 27.163 | 1.00 31.64 |
| ATOM | 3292 | N | ALA | 473 | -10.702 | 33.067 31.790 | 25.252 | 1.00 31.77 1.00 32.34 |
| ATOM ATOM | 3293 3294 | CA CB | ALA ALA | 473 473 | -10.297 -9.802 | 30.850 | 25.840 24.743 | 1.00 32.34 |
| ATOM | 3295 | C | ALA | 473 | -9.222 | 31.946 | 26.915 | 1.00 32.08 |
| ATOM | 3296 | ō | ALA | 473 | -9.133 | 31.132 | 27.835 | 1.00 32.20 |
| MOTA | 3297 | N | GLY | 474 | -8.401 | 32.987 | 26.793 | 1.00 32.17 |
| MOTA | 3298 | CA | GLY | 474 | -7.352 | 33.217 | 27.774 | 1.00 32.43 |
| MOTA | 3299 | C | GLY | 474 | -5.991 | 33.553 | 27.182 | 1.00 33.77 |
| ATOM | 3300 | 0 | GLY | 474 | -5.027 | 33.776 | 27.916 | 1.00-32.28 |
| MOTA | 3301 | N | ALA | 475 | -5.905 | 33.589 | 25.856 | 1.00 34.78 |
| MOTA | 3302 | CA | ALA | 475 475 | -4.646 | 33.905 33.850 | 25.189 23.679 | 1.00 36.82 1.00 37.72 |
| ATOM ATOM | 3303 3304 | CB C | ALA ALA | 475 | -4.820 -4.170 | 35.289 | 25.608 | 1.00 37.72 1.00 38.74 |
| ATOM | 3305 | 0 | ALA | 475 | -4.896 | 36.276 | 25.466 | 1.00 38.36 |
| ATOM | 3306 | N | GLN | 476 | -2.947 | 35.354 | 26.124 | 1.00 39.30 |
| ATOM | 3307 | CA | GLN | 476 | -2.370 | 36.618 | 26.573 | 1.00 41.42 |
| ATOM | 3308 | CB | GLN | 476 | -1.484 | 36.378 | 27.798 | 1.00 42.23 |
| MOTA | 3309 | CG, | GLN | 476 | -2.195 | 35.668 | 28.940 | 1.00 44.93 |
| MOTA | 3310 | CD | GLN | 476 | -1.408 | 35.724 | 30.234 | 1.00 46.68 |
| MOTA | | OE1 | | 476 | -1.176 | 36.802 | 30.780 | 1.00 48.89 |
| ATOM | 3312 3313 | NE2 C | GLN | 476 476 | -0.992 -1.561 | 34.564 37.296 | | 1.00 47.84 1.00 41.29 |
| ATOM ATOM | 3314 | 0 | ~ | 476 | -1.171 | 38.459 | 25.590 | 1.00 41.29 |
| ATOM | 3315 | N | LEU | 477 | -1.320 | 36.558 | 24.389 | 1.00 40.91 |
| MOTA | 3316 | CA | LEU | 477 | -0.565 | 37.058 | 23.247 | 1.00 39.33 |
| ATOM | 3317 | CB | LEU | 477 | 0.915 | 36.716 | 23.395 | 1.00 41.45 |
| ATOM | 3318 | CG | LEU | 477 | 1.785 | 37.738 | 24.121 | 1.00 41.89 |
| MOTA | 3319 | CD1 | | 477 | 3.142 | 37.133 | 24.420 | 1.00 42.32 |
| MOTA | 3320 | CD2 | | 477 | 1.927 | 38.977 | 23.252 | 1.00 43.54 |
| MOTA | 3321 | C | LEU | 477 477 | -1.086 -1.714 | 36.455 35.400 | 21.953 21.964 | 1.00 38.33 1.00 36.02 |
| MOTA MOTA | 3322 3323 | O N | LEU LEU | 478 | -0.820 | 37.130 | 20.840 | 1.00 36.02 |
| MOTA | 3324 | | LEU | 478 | -1.258 | 36.659 | 19.533 | 1.00 38.87 |
| ATOM | 3325 | СВ | LEU | 478 | -2.600 | 37.288 | 19.158 | 1.00 38.65 |
| MOTA | 3326 | CG · | LEU | 478 | -3.100 | 36.978 | 17.748 | 1.00 40.05 |
| MOTA | 3327 | CD1 | LEU | 478 | -3.361 | 35.488 | 17.611 | 1.00 39.92 |
| MOTA | 3328 | CD2 | | 478 | -4.369 | 37.771 | 17.467 | 1.00 40.39 |
| ATOM | 3329 | C | LEU | 478 | -0.227 | 37.002 | 18.465 | 1.00 38.90 |
| ATOM | 3330 | 0 | LEU | 478 | 0.424 | 38.047 | 18.528 | 1.00 39.77 |
| ATOM ATOM | 3331 3332 | N CA | VAL VAL | 479 479 | -0.084 0.862 | 36.120 36.337 | 17.483 16.402 | 1.00 38.07 1.00 37.86 |
| ATOM | 3333 | CB | VAL | 479 | 2.033 | 35.332 | 16.478 | 1.00 37.86 |
| ATOM | 3334 | | VAL | 479 | 2.952 | 35.503 | 15.284 | 1.00 37.71 |
| ATOM | 3335 | | VAL | 479 | 2.808 | 35.537 | 17.771 | 1.00 37.24 |
| ATOM | 3336 | C | VAL | 479 | 0.174 | 36.200 | 15.049 | 1.00 39.03 |
| | 3337 | 0 | VAL | 479 | -0.453 | 35.176 | 14.760 | 1.00 37.57 |
| ATOM | 3338 | N · | | 480 | 0.282 | 37.246 | 14.231 | 1.00 38.25 |
| ATOM | 3339 | CA | LEU | 480 | -0.307 | 37.251 | 12.893 | 1.00 38.69 |

| АТОМ | 3340 | СВ | LEU | 480 | -1.029 | 38.574 | 12.622 | 1.00 39.15 |
|--------------|--------------|-----------|------------|------------|------------------|------------------|------------------|--------------------------|
| ATOM | 3341 | CG | LEU | 480 | -2.307 | 38.841 | 13.418 | 1.00 39.59 |
| MOTA | 3342 | CD1 | | 480 | -2.851 | 40.220 | 13.071 | 1.00 39.86 |
| ATOM | 3343 | CD2 | | 480 | -3.340 | 37.766 | 13.098 | 1.00 40.86 |
| MOTA | 3344 3345 | С | LEU | 480 480 | 0.816 | 37.067 | 11.884 | 1.00 38.26 1.00 37.03 |
| ATOM ATOM | 3345 | O N | LEU GLU | 480 | 1.818 0.648 | 37.776 36.115 | 11.935 10.972 | 1.00 37.03 |
| ATOM | 3347 | CA | GLU | 481 | 1.670 | 35.846 | 9.967 | 1.00 38.65 |
| ATOM | 3348 | СВ | GLU | 481 | 2.287 | 34.469 | 10.204 | 1.00 38.33 |
| ATOM | 3349 | CG | GLU | 481 | 3.587 | 34.243 | 9.454 | 1.00 39.77 |
| ATOM | 3350 | CD | GLU | 481 | 4.111 | 32.833 | 9.611 | 1.00 38.78 |
| MOTA | 3351 | OE1 | | 481 | 4.045 | 32.300 | 10.741 | 1.00 36.25 |
| ATOM | 3352 | OE2 | | 481 | 4.597 | 32.266 | 8.605 | 1.00 39.84 1.00 39.06 |
| ATOM ATOM | 3353 3354 | C 0 | GLU | 481 481 | 1.123 0.152 | 35.914 35.234 | 8.546 8.209 | 1.00 37.10 |
| ATOM | 3355 | N | CYS | 482 | 1.768 | 36.732 | 7.719 | 1.00 41.00 |
| ATOM | 3356 | CA | CYS | 482 | 1.384 | 36.918 | 6.323 | 1.00 42.86 |
| ATOM | 3357 | СВ | CYS | 482 | 1.841 | 35.721 | 5.490 | 1.00 42.97 |
| ATOM | 3358 | SG | CYS | 482 | 3.640 | 35.526 | 5.444 | 1.00 44.40 |
| ATOM | 3359 | C | CYS | 482 | -0.110 | 37.139 | 6.142 | 1.00 43.47 |
| ATOM | 3360 | Ο. | CYS | 482 | -0.829 | 36.260 | 5.664 | 1.00 44.42 |
| ATOM ATOM | 3361 3362 | N CA | VAL VAL | 483 483 | -0.564 -1.969 | 38.327 38.697 | 6.524 6.411 | 1.00 45.25 1.00 47.42 |
| ATOM | 3363 | CB | VAL | 483 | -2.682 | 38.573 | 7.783 | 1.00 47.42 |
| ATOM | 3364 | CG1 | | 483 | -2.199 | 39.655 | 8.730 | 1.00 47.74 |
| MOTA | 3365 | CG2 | VAL | 483 | -4.182 | 38.643 | 7.603 | 1.00 48.49 |
| MOTA | 3366 | С | VAL | 483 | -2.053 | 40.143 | 5.915 | 1.00 48.82 |
| MOTA | 3367 | 0 | VAL | 483 | -1.243 | 40.987 | 6.304 | 1.00 49.32 |
| ATOM | 3368 | N | PRO | 484 | -3.027 -4.159 | 40.449 39.629 | 5.042 4.579 | 1.00 49.61 1.00 50.26 |
| ATOM ATOM | 3369 3370 | CD CA | PRO PRO | 484 484 | -3.143 | 41.822 | 4.541 | 1.00 49.54 |
| ATOM | 3371 | CB | PRO | 484 | -4.459 | 41.797 | 3.758 | 1.00 49.60 |
| ATOM | 3372 | CG | PRO | 484 | -5.229 | 40.670 | 4.391 | 1.00 50.57 |
| MOTA | 3373 | С | PRO | 484 | -3.138 | 42.850 | 5.666 | 1.00 49.40 |
| MOTA | 3374 | 0 | PRO | 484 | -3.852 | 42.703 | 6.656 | 1.00 49.27 |
| ATOM | 3375 | N | VAL | 485 | -2.317 | 43.884 | 5.504 | 1.00 49.36 |
| MOTA | 3376 3377 | CA | VAL VAL | 485 485 | -2.184 -1.436 | 44.942 46.156 | 6.500 5.915 | 1.00 49.33 1.00 48.81 |
| ATOM ATOM | 3378 | CB CG1 | | 485 | -1.169 | 47.171 | 7.006 | 1.00 49.88 |
| ATOM | 3379 | CG2 | | 485 | -0.134 | 45.707 | 5.273 | 1.00 49.01 |
| MOTA | 3380 | С | VAL | 485 | -3.532 | 45.415 | 7.034 | 1.00 50.17 |
| MOTA | 3381 | 0 | VAL | 485 | -3.732 | 45.505 | 8.248 | 1.00 49.86 |
| MOTA | 3382 | N | GLU | 486 | -4.454 | 45.715 | 6.124 | 1.00 50.05 |
| ATOM | 3383 | CA | GLU | 486 | -5.784 -6.644 | 46.183 46.421 | 6.504 5.254 | 1.00 50.38 1.00 51.37 |
| ATOM ATOM | 3384 3385 | CB CG | GLU GLU | 486 486 | -6.277 | 45.568 | 4.041 | 1.00 52.69 |
| ATOM | 3386 | CD | GLU | 486 | -5.076 | 46.115 | 3.277 | 1.00 53.84 |
| MOTA | 3387 | OE1 | | 486 | -5.120 | 47.296 | 2.872 | 1.00 54.68 |
| MOTA | 3388 | OE2 | GLU | 486 | -4.096 | 45.365 | 3.074 | 1.00 52.54 |
| MOTA | 3389 | С | GLU | 486 | -6.503 | 45.228 | 7.456 | 1.00 50.03 |
| ATOM | 3390 | 0 | GLU | 486 | -7.304 | 45.656 43.936 | 8.292 | 1.00 48.95 |
| MOTA | 3391 3392 | N CA | LEU | 487 487 | -6.215 -6.837 | 43.936 | 7.330 8.187 | 1.00 49.68 1.00 50.28 |
| ATOM ATOM | 3393 | CB | LEU | 487 | -6.709 | 41.543 | 7.553 | 1.00 50.28 |
| ATOM | 3394 | CG | LEU | 487 | -7.813 | 40.529 | 7.871 | 1.00 52.57 |
| MOTA | 3395 | CD1 | LEU | 487 | -7.551 | 39.250 | 7.099 | 1.00 53.26 |
| MOTA | 3396 | | LEU | 487 | -7.875 | 40.253 | 9.361 | 1.00 53.45 |
| MOTA | 3397 | C . | LEU | 487 | -6.158 | 42.948 | 9.556 | 1.00 49.71 |
| ATOM | 3398 | O N | LEU ALA | 487 488 | -6.811 -4.841 | 42.801 43.128 | 10.591 9.549 | 1.00 48.49 1.00 49.21 |
| ATOM ATOM | 3399 3400 | CA | ALA | 488 | -4.071 | 43.177 | 10.784 | 1.00 48.39 |
| ATOM | 3401 | СВ | ALA | 488 | -2.583 | 43.275 | 10.468 | 1.00 48.13 |
| MOTA | 3402 | С | ALA | 488 | -4.513 | 44.380 | 11.607 | 1.00 48.23 |
| MOTA | 3403 | 0 | ALA | 488 | -4.465 | 44.353 | 12.835 | 1.00 48.24 |
| MOTA | 3404 | N | LYS | 489 | -4.946 | 45.433 | 10.923 | 1.00 48.36 |
| ATOM | 3405 | CA | LYS | 489 489 | -5.399 -5.738 | 46.646 47.721 | 11.593 10.564 | 1.00 48.70 1.00 49.47 |
| ATOM ATOM | 3406 3407 | CB CG | LYS LYS | 489 | -4.615 | 48.018 | 9.591 | 1.00 49.47 |
| ATOM | 3408 | CD | LYS | 489 | -5.070 | 48.969 | 8.495 | 1.00 53.59 |
| ATOM | 3409 | CE | LYS | 489 | -3.995 | 49.127 | 7.431 | 1.00 54.03 |
| MOTA | 3410 | NZ | LYS | 489 | -4.460 | 49.959 | 6.292 | 1.00 54.51 |
| MOTA | 3411 | C | LYS | 489 | -6.626 | 46.357 | 12.450 | 1.00 48.17 |
| ATOM | 3412 | 0 | LYS | 489 | -6.667 -7.627 | 46.723 | 13.623 | 1.00 47.72 1.00 48.64 |
| ATOM ATOM | 3413 3414 | N CA | ARG ARG | 490 490 | -7.627 -8.842 | 45.704 45.377 | 11.863 12.605 | 1.00 48.84 |
| ATOM | 3415 | CB | ARG | 490 | -9.846 | 44.622 | 11.725 | 1.00 49.59 |
| ATOM | 3416 | CG | ARG | 490 | -10.743 | 45.511 | 10.884 | 1.00 50.73 |

| ATOM | 3417 | CD | ARG | 490 | -12.089 | 44.836 | 10.629 | 1.00 51.13 |
|--------|------|-----|-----|-------|---------|--------|--------|------------|
| ATOM | 3418 | NE | ARG | 490 | -11.966 | 43.619 | 9.832 | 1.00 51.85 |
| ATOM | 3419 | CZ | ARG | 490 | -12.959 | 42.759 | 9.616 | 1.00 51.49 |
| ATOM | 3420 | NH1 | | 490 | -14.157 | 42.977 | 10.141 | 1.00 51.44 |
| | 3421 | | ARG | 490 | -12.755 | 41.680 | 8.871 | 1.00 50.98 |
| ATOM | | | | | | 44.532 | | 1.00 48.05 |
| MOTA | 3422 | С | ARG | 490 | -8.525 | | 13.831 | |
| ATOM | 3423 | 0 | ARG | 490 | -8.860 | 44.904 | 14.956 | 1.00 48.14 |
| MOTA | 3424 | N | ILE | 491 | -7.874 | 43.394 | 13.603 | 1.00 47.40 |
| MOTA | 3425 | CA | ILE | 491 | -7.509 | 42.477 | 14.679 | 1.00 46.20 |
| MOTA | 3426 | CB | ILE | 491 | -6.621 | 41.323 | 14.150 | 1.00 45.42 |
| ATOM | 3427 | CG2 | ILE | 491 | -6.168 | 40.440 | 15.304 | 1.00 45.08 |
| ATOM | 3428 | CG1 | ILE | 491 | -7.403 | 40.494 | 13.126 | 1.00 45.31 |
| ATOM . | 3429 | CD1 | ILE | 491 | -6.608 | 39.364 | 12.503 | 1.00 45.50 |
| ATOM | 3430 | С | ILE | 491 | -6.777 | 43.188 | 15.811 | 1.00 45.67 |
| ATOM | 3431 | 0 | ILE | 491 | -7.119 | 43.022 | 16.982 | 1.00 45.67 |
| ATOM | 3432 | N | THR | 492 | -5.773 | 43.984 | 15.460 | 1.00 45.88 |
| ATOM | 3433 | CA | THR | 492 | -4.998 | 44.715 | 16.456 | 1.00 45.57 |
| ATOM | 3434 | CB | THR | 492 | -3.790 | 45.421 | 15.814 | 1.00 44.78 |
| ATOM | 3435 | OG1 | | 492 | -3.046 | 44.481 | 15.030 | 1.00 44.42 |
| | | | | | | | 16.891 | 1.00 43.82 |
| ATOM | 3436 | | THR | 492 | -2.882 | 46.000 | | |
| ATOM | 3437 | C | THR | 492 | -5.849 | 45.768 | 17.155 | 1.00 46.83 |
| ATOM | 3438 | 0 | THR | 492 | -5.732 | 45.968 | 18.366 | 1.00 47.12 |
| ATOM | 3439 | N | GLU | 493 | -6.699 | 46.444 | 16.387 | 1.00 47.21 |
| MOTA | 3440 | CA | GLU | 493 | -7.568 | 47.483 | 16.934 | 1.00 48.40 |
| ATOM | 3441 | CB | GLU | 493 | -7.898 | 48.523 | 15.860 | 1.00 49.93 |
| ATOM | 3442 | CG | GLU | 493 | -6.713 | 49.354 | 15.407 | 1.00 52.65 |
| MOTA | 3443 | CD | GLU | 493 | -7.088 | 50.372 | 14.347 | 1.00 54.51 |
| ATOM | 3444 | OE1 | GLU | 493 | -7.493 | 49.957 | 13.238 | 1.00 55.78 |
| ATOM | 3445 | QE2 | GLU | 493 | -6.980 | 51.585 | 14.623 | 1.00 55.00 |
| MOTA | 3446 | С | GLU | 493 | -8.866 | 46.909 | 17.486 | 1.00 47.51 |
| ATOM | 3447 | 0 | GLU | 493 | -9.806 | 47.651 | 17.776 | 1.00 48.38 |
| ATOM - | 3448 | N | ALA | 494 | -8.914 | 45.587 | 17.630 | 1.00 45.76 |
| ATOM | 3449 | CA | ALA | 494 | -10.103 | 44.916 | 18.143 | 1.00 43.41 |
| ATOM | 3450 | СВ | ALA | 494 | -10.674 | 43.983 | 17.081 | 1.00 43.68 |
| ATOM | 3451 | C | ALA | 494 | -9.790 | 44.129 | 19.407 | 1.00 41.36 |
| | 3452 | 0 | | 494 | -10.674 | 43.879 | 20.226 | 1.00 40.45 |
| ATOM | | | ALA | | | 43.741 | | 1.00 40.45 |
| ATOM | 3453 | N | LEU | 495 | -8.528 | | 19.559 | |
| ATOM | 3454 | CA | LEU | 495 | -8.103 | 42.974 | 20.723 | 1.00 37.83 |
| ATOM | 3455 | CB | LEU | 495 | -7.126 | 41.866 | 20.310 | 1.00 37.72 |
| MOTA | 3456 | CG | LEU | 495 | -7.606 | 40.812 | 19.305 | 1.00 38.81 |
| ATOM | 3457 | | LEU | 495 | -6.498 | 39.797 | 19.069 | 1.00 37.67 |
| ATOM | 3458 | | LEU | 495 | -8.851 | 40.121 | 19.825 | 1.00 39.75 |
| MOTA | 3459 | С | LEU | 495 | -7.446 | 43.851 | 21.780 | 1.00 37.16 |
| MOTA | 3460 | 0 | LEU | 495 | -6.866 | 44.895 | 21.473 | 1.00 35.11 |
| MOTA | 3461 | N | ALA | 496 | -7.542 | 43.414 | 23.031 | 1.00 36.75 |
| ATOM | 3462 | CA | ALA | 496 | -6.954 | 44.141 | 24.143 | 1.00 37.22 |
| ATOM | 3463 | CB | ALA | 496 | -7.780 | 43.927 | 25.399 | 1.00 36.82 |
| ATOM | 3464 | С | ALA | 496 | -5.527 | 43.656 | 24.360 | 1.00 37.76 |
| ATOM | 3465 | 0 | ALA | 496 | -4.656 | 44.427 | 24.754 | 1.00 38.66 |
| ATOM | 3466 | N | ILE | 497 | -5.291 | 42.374 | 24.097 | 1.00 38.35 |
| ATOM | 3467 | CA | ILE | 497 | -3.961 | 41.793 | 24.263 | 1.00 38.83 |
| ATOM | 3468 | СВ | ILE | 497 | -4.015 | 40.246 | 24.284 | 1.00 37.92 |
| ATOM | 3469 | CG2 | ILE | 497 | -4.894 | 39.770 | 25.438 | 1.00 37.32 |
| ATOM | 3470 | CG1 | ILE | 497 | -4.558 | 39.728 | 22.950 | 1.00 38.42 |
| ATOM | 3471 | CD1 | ILE | 497 | -4.531 | 38.220 | 22.814 | 1.00 38.06 |
| ATOM | 3472 | C | ILE | 497 | -3.052 | 42.220 | 23.117 | 1.00 39.35 |
| ATOM | 3473 | 0 | ILE | 497 | -3.517 | 42.443 | 21.998 | 1.00 40.82 |
| | | | | | | | 23.377 | |
| ATOM | 3474 | N | PRO | 498 | -1.739 | 42.333 | | 1.00 39.89 |
| ATOM | 3475 | CD | PRO | 498 | -1.048 | 42.058 | 24.648 | 1.00 38.22 |
| ATOM | 3476 | CA | PRO | 498 | -0.786 | 42.737 | 22.336 | 1.00 39.86 |
| ATOM | 3477 | СВ | PRO | 498 | 0.541 | 42.807 | 23.093 | 1.00 40.07 |
| ATOM | 3478 | CG | PRO | 498 | 0.359 | 41.804 | 24.190 | 1.00 39.95 |
| ATOM | 3479 | C | PRO | 498 | -0.745 | 41.764 | 21.158 | 1.00 40.23 |
| ATOM | 3480 | 0 | PRO | 498 | -0.824 | 40.551 | 21.341 | 1.00 40.13 |
| MOTA | 3481 | N | VAL | 499 | -0.631 | 42.302 | 19.947 | 1.00 40.04 |
| MOTA | 3482 | ·CA | VAL | 499 | -0.588 | 41.475 | 18.746 | 1.00 39.96 |
| MOTA | 3483 | CB | VAL | 499 . | -1.711 | 41.877 | 17.754 | 1.00 39.82 |
| MOTA | 3484 | CG1 | VAL | 499 | -1.678 | 40.978 | 16.527 | 1.00 39.71 |
| MOTA | 3485 | CG2 | VAL | 499 | -3.068 | 41.785 | 18,440 | 1.00 39.57 |
| ATOM | 3486 | С | VAL | 499 | 0.762 | 41.592 | 18.040 | 1.00 40.53 |
| | 3487 | 0 | VAL | 499 | 1.081 | 42.633 | 17.468 | 1.00 40.65 |
| MOTA | 3488 | N | ILE | 500 | 1.555 | 40.524 | 18.089 | 1.00 41.28 |
| ATOM | 3489 | CA | ILE | 500 | 2.865 | 40.509 | 17.444 | 1.00 41.57 |
| ATOM | 3490 | СВ | ILE | 500 | 3.828 | 39.525 | 18.142 | 1.00 42.09 |
| ATOM | 3491 | CG2 | ILE | 500 | 5.176 | 39.522 | 17.429 | 1.00 42.77 |
| ATOM | 3492 | CG1 | ILE | 500 | 4.006 | 39.927 | 19.608 | 1.00 43.30 |
| ATOM | 3493 | CD1 | | 500 | 4.799 | 38.930 | 20.434 | 1.00 43.71 |
| | | | | | | 50.550 | | 45.71 |

| 3 mon | 3494 | С | ILE | 500 | 2.695 | 40.090 | 15.990 | 1 00 | 41.61 |
|-------|------|-----------|-----|-----|--------|--------|--------|------|-------|
| ATOM | | | | | | | | | |
| ATOM | 3495 | 0 | ILE | 500 | 2.071 | 39.068 | 15.693 | 1.00 | 40.85 |
| MOTA | 3496 | N | GLY | 501 | 3.254 | 40.881 | 15.081 | | 40.82 |
| MOTA | 3497 | CA | GLY | 501 | 3.118 | 40.572 | 13.672 | | 40.29 |
| MOTA | 3498 | С | GLY | 501 | 4.371 | 40.098 | 12.968 | 1.00 | 39.63 |
| ATOM | 3499 | 0 | GLY | 501 | 5.494 | 40.348 | 13.405 | 1.00 | 39.28 |
| ATOM | 3500 | N | ILE | 502 | 4.154 | 39.401 | 11.860 | 1.00 | 39.72 |
| | 3501 | CA | ILE | 502 | 5.226 | 38.875 | 11.032 | | 41.34 |
| MOTA | | | | | | | | | |
| MOTA | 3502 | СВ | ILE | 502 | 5.709 | 37.488 | 11.553 | | 41.52 |
| MOTA | 3503 | CG2 | ILE | 502 | 4.522 | 36.582 | 11.830 | | 42.33 |
| MOTA | 3504 | CG1 | ILE | 502 | 6.659 | 36.845 | 10.544 | 1.00 | 42.33 |
| MOTA | 3505 | CD1 | ILE | 502 | 7.958 | 37.584 | 10.375 | 1.00 | 43.95 |
| ATOM | 3506 | C | ILE | 502 | 4.676 | 38.766 | 9.609 | 1.00 | 42.06 |
| ATOM | 3507 | ō | ILE | 502 | 4.029 | 37.782 | 9.245 | | 42.10 |
| | | | GLY | 503 | 4.922 | 39.801 | 8.812 | | 43.11 |
| ATOM | 3508 | N | | | | | | | |
| MOTA | 3509 | CA | GLY | 503 | 4.426 | 39.817 | 7.449 | | 44.13 |
| ATOM | 3510 | C | GLY | 503 | 2.981 | 40.273 | 7.444 | | 44.13 |
| ATOM | 3511 | 0 | GLY | 503 | 2.215 | 39.950 | 6.535 | 1.00 | 44.93 |
| ATOM | 3512 | N | ALA | 504 | 2.612 | 41.028 | 8.474 | 1.00 | 44.37 |
| ATOM | 3513 | CA | ALA | 504 | 1.255 | 41.540 | 8.610 | 1.00 | 45.44 |
| ATOM | 3514 | СВ | ALA | 504 | 0.612 | 40.976 | 9.871 | | 45.34 |
| ATOM | 3515 | C | ALA | 504 | 1.249 | 43.065 | 8.663 | | 45.59 |
| | | | | 504 | | | 9.026 | | 45.09 |
| ATOM | 3516 | 0 | ALA | | 0.245 | 43.677 | | | |
| MOTA | 3517 | N | GLY | 505 | 2.373 | 43.672 | 8.296 | | 46.27 |
| MOTA | 3518 | CA | GLY | 505 | 2.465 | 45.119 | 8.316 | | 47.16 |
| MOTA | 3519 | С | GLY | 505 | 2.955 | 45.644 | 9.652 | | 47.80 |
| ATOM | 3520 | 0 | GLY | 505 | 3.187 | 44.870 | 10.581 | 1.00 | 46.72 |
| MOTA | 3521 | N | ASN | 506 | 3.106 | 46.963 | 9.749 | 1.00 | 47.19 |
| ATOM | 3522 | CA | ASN | 506 | 3.582 | 47.600 | 10.974 | | 47.23 |
| | | | ASN | 506 | 4.561 | 48.725 | 10.624 | | 47.68 |
| ATOM | 3523 | CB | | | | | | | |
| MOTA | 3524 | CG | ASN | 506 | 3.972 | 49.737 | 9.656 | | 47.63 |
| MOTA | 3525 | OD1 | ASN | 506 | 4.678 | 50.613 | 9.156 | | 49.34 |
| MOTA | 3526 | ND2 | ASN | 506 | 2.676 | 49.623 | 9.388 | 1.00 | 47.05 |
| ATOM | 3527 | С | ASN | 506 | 2.445 | 48.146 | 11.836 | 1.00 | 47.02 |
| ATOM | 3528 | 0 | ASN | 506 | 2.671 | 48.962 | 12.734 | 1.00 | 45.93 |
| ATOM | 3529 | N | VAL | 507 | 1.229 | 47.681 | 11.561 | | 46.55 |
| ATOM | 3530 | CA | VAL | 507 | 0.046 | 48.106 | 12.300 | | 46.94 |
| | | | | | | | | | 47.55 |
| ATOM | 3531 | CB | VAL | 507 | -1.238 | 47.855 | 11.482 | | |
| ATOM | 3532 | CG1 | VAL | 507 | -2.447 | 48.398 | 12.228 | | 48.40 |
| MOTA | 3533 | CG2 | VAL | 507 | -1.117 | 48.506 | 10.117 | | 48.35 |
| ATOM | 3534 | C | VAL | 507 | -0.070 | 47.357 | 13.622 | 1.00 | 46.72 |
| ATOM | 3535 | 0 | VAL | 507 | -0.693 | 47.842 | 14.567 | 1.00 | 47.09 |
| ATOM | 3536 | N | THR | 508 | 0.531 | 46.171 | 13.683 | 1.00 | 46.59 |
| ATOM | 3537 | CA | THR | 508 | 0.494 | 45.355 | 14.896 | | 46.09 |
| | | CB | | 508 | 1.109 | 43.955 | 14.653 | 1.00 | |
| ATOM | 3538 | | THR | | | | | | |
| MOTA | 3539 | OG1 | THR | 508 | 2.438 | 44.091 | 14.138 | | 46.20 |
| MOTA | 3540 | CG2 | THR | 508 | 0.264 | 43.166 | 13.658 | | 45.82 |
| MOTA | 3541 | С | THR | 508 | 1.239 | 46.036 | 16.042 | | 45.51 |
| ATOM | 3542 | 0 | THR | 508 | 2.017 | 46.964 | 15.823 | 1.00 | 45.43 |
| ATOM | 3543 | N | ASP | 509 | 0.993 | 45.572 | 17.263 | 1.00 | 44.71 |
| MOTA | 3544 | CA | ASP | 509 | 1.630 | 46.140 | 18.447 | 1.00 | 44.33 |
| ATOM | 3545 | CB | ASP | 509 | 0.940 | 45.627 | 19.713 | | 43.80 |
| | | | | 509 | -0.541 | 45.942 | 19.738 | | 43.81 |
| ATOM | 3546 | CG OD1 | ASP | 509 | -0.899 | 47.139 | 19.730 | | 41.97 |
| ATOM | 3547 | | ASP | | | | | | |
| MOTA | 3548 | | ASP | 509 | -1.349 | 44.990 | 19.764 | | 44.48 |
| MOTA | 3549 | C | ASP | 509 | 3.113 | 45.801 | 18.510 | | 44.55 |
| ATOM | 3550 | 0 | ASP | 509 | 3.914 | 46.576 | 19.030 | | 44.42 |
| MOTA | 3551 | N | GLY | 510 | 3.473 | 44.636 | 17.983 | | 44.35 |
| ATOM | 3552 | CA | GLY | 510 | 4.864 | 44.225 | 18.001 | 1.00 | 44.15 |
| MOTA | 3553 | С | GLY | 510 | 5.269 | 43.479 | 16.749 | 1.00 | 44.41 |
| ATOM | 3554 | ō | GLY | 510 | 4.445 | 43.221 | 15.870 | | 45.25 |
| ATOM | | | | 511 | 6.547 | 43.129 | 16.667 | | 43.48 |
| | 3555 | N | GLN | | | | | | 42.71 |
| ATOM | 3556 | CA | GLN | 511 | 7.063 | 42.406 | 15.513 | | |
| ATOM | 3557 | CB | GLN | 511 | 7.893 | 43.342 | 14.625 | | 42.63 |
| MOTA | 3558 | CG | GLN | 511 | 7.109 | 44.465 | 13.958 | | 39.39 |
| MOTA | 3559 | CD | GLN | 511 | 6.088 | 43.957 | 12.959 | | 38.03 |
| MOTA | 3560 | OE1 | GLN | 511 | 6.386 | 43.093 | 12.136 | 1.00 | 36.45 |
| ATOM | 3561 | NE2 | GLN | 511 | 4.878 | 44.502 | 13.017 | 1.00 | 37.24 |
| ATOM | 3562 | C | GLN | 511 | 7.930 | 41.238 | 15.959 | | 43.26 |
| | | - | | 511 | 8.402 | 41.197 | 17.094 | | 42.66 |
| ATOM | 3563 | 0 | GLN | | | 40.287 | 15.055 | | 43.65 |
| ATOM | 3564 | N | ILE | 512 | 8.130 | | | | |
| ATOM | 3565 | CA | ILE | 512 | 8.957 | 39.125 | 15.343 | | 44.30 |
| MOTA | 3566 | CB | ILE | 512 | 8.159 | 38.052 | 16.124 | | 43.90 |
| MOTA | 3567 | CG2 | ILE | 512 | 7.079 | 37.448 | 15.234 | | 44.70 |
| MOTA | 3568 | CG1 | ILE | 512 | 9.108 | 36.962 | 16.627 | | 43.78 |
| MOTA | 3569 | | ILE | 512 | 8.463 | 35.995 | 17.595 | 1.00 | 43.66 |
| ATOM | 3570 | C | ILE | 512 | 9.472 | 38.536 | 14.028 | | 44.66 |
| | | _ | | | | | | | |

| ATOM | 3571 | 0 | ILE | 512 | 8.843 | 38.689 | 12.979 | 1.00 44.73 |
|------|----------------|-----|-----|-----|--------|--------|----------|------------|
| ATOM | 3572 | N | LEU | 513 | 10.625 | 37.879 | 14.087 | 1.00 45.11 |
| MOTA | 3573 | CA | LEU | 513 | 11.215 | 37.274 | 12.903 | 1.00 45.41 |
| | | | LEU | 513 | 11.690 | 38.360 | 11.936 | 1.00 47.61 |
| ATOM | 3574 | CB | | | | | | |
| ATOM | 3575 | CG | LEU | 513 | 11.333 | 38.180 | 10.457 | 1.00 49.48 |
| ATOM | 3576 | CD1 | | 513 | 12.121 | 39.187 | 9.645 | 1.00 50.43 |
| ATOM | 3577 | CD2 | LEU | 513 | 11.651 | 36.759 | 9.988 | 1.00 50.20 |
| MOTA | 3578 | С | LEU | 513 | 12.400 | 36.396 | 13.288 | 1.00 44.78 |
| ATOM | 3579 | 0 | LEU | 513 | 13.020 | 36.594 | 14.337 | 1.00 44.20 |
| ATOM | 3580 | N | VAL | 514 | 12.714 | 35.428 | 12.432 | 1.00 43.32 |
| ATOM | 3581 | CA | VAL | 514 | 13.834 | 34.532 | 12.683 | 1.00 43.17 |
| ATOM | 3582 | CB | VAL | 514 | 13.914 | 33.413 | 11.623 | 1.00 43.69 |
| ATOM | 3583 | CG1 | VAL | 514 | 15.057 | 32.460 | 11.960 | 1.00 43.51 |
| | | CG2 | | | | 32.669 | | 1.00 43.46 |
| MOTA | 3584 | | VAL | 514 | 12.594 | | 11.554 | |
| ATOM | 3585 | C | VAL | 514 | 15.124 | 35.342 | 12.638 | 1.00 42.43 |
| MOTA | 3586 | 0 | VAL | 514 | 15.377 | 36.069 | 11.679 | 1.00 42.48 |
| MOTA | 3587 | N | MET | 515 | 15.931 | 35.214 | 13.684 | 1.00 41.21 |
| MOTA | 3588 | CA | MET | 515 | 17.190 | 35.935 | 13.772 | 1.00 40.22 |
| ATOM | 3589 | CB | MET | 515 | 17.929 | 35.543 | 15.050 | 1.00 38.49 |
| MOTA | 3590 | CG | MET | 515 | 18.189 | 34.057 | 15.180 | 1.00 37.77 |
| ATOM | 3591 | SĐ | MET | 515 | 19.693 | 33.741 | 16.107 | 1.00 37.43 |
| ATOM | 3592 | CE | MET | 515 | 20.902 | 33.853 | 14.776 | 1.00 39.24 |
| MOTA | 3593 | С | MET | 515 | 18.086 | 35.669 | 12.569 | 1.00 40.31 |
| MOTA | 3594 | ō | MET | 515 | 18.749 | 36.575 | 12.063 | 1.00 39.94 |
| ATOM | 3595 | N | HIS | 516 | 18.100 | 34.420 | 12.116 | 1.00 40.39 |
| | 3596 | | HIS | | | | | 1.00 40.39 |
| ATOM | | CA | | 516 | 18.916 | 34.011 | 10.978 | |
| ATOM | 3597 | CB | HIS | 516 | 18.683 | 32.523 | 10.694 | 1.00 40.66 |
| MOTA | 3598 | CG | HIS | 516 | 19.230 | 31.619 | 11.755 | 1.00 39.06 |
| MOTA | 3599 | | HIS | 516 | 18.682 | 31.162 | 12.906 | 1.00 37.78 |
| MOTA | 3600 | ND1 | HIS | 516 | 20.517 | 31.128 | 11.725 | 1.00 38.08 |
| MOTA | 3601 | | HIS | 516 | 20.740 | 30.409 | 12.810 | 1.00 35.88 |
| ATOM | 3602 | NE2 | HIS | 516 | 19.642 | 30.415 | 13.544 | 1.00 37.95 |
| ATOM | 3603 | С | HIS | 516 | 18.657 | 34.836 | 9.718 | 1.00 42.74 |
| ATOM | 3604 | 0 | HIS | 516 | 19.558 | 35.025 | 8.898 | 1.00 42.29 |
| ATOM | 3605 | N | ASP | 517 | 17.429 | 35.323 | 9.567 | 1.00 43.70 |
| ATOM | 3606 | CA | ASP | 517 | 17.064 | 36.134 | 8.410 | 1.00 45.81 |
| MOTA | 3607 | СВ | ASP | 517 | 15.640 | 35.807 | 7.953 | 1.00 45.49 |
| ATOM | 3608 | CG | ASP | 517 | 15.572 | 34.538 | 7.124 | 1.00 47.31 |
| | | | | | | | | |
| MOTA | 3609 | | ASP | 517 | 16.287 | 34.456 | 6.104 | 1.00 47.95 |
| MOTA | 3610 | OD2 | ASP | 517 | 14.803 | 33.627 | 7.481 | 1.00 48.46 |
| MOTA | 3611 | С | ASP | 517 | 17.175 | 37.625 | 8.708 | 1.00 46.65 |
| ATOM | 3612 | 0 | ASP | 517 | 17.175 | 38.452 | 7.794 | 1.00 47.65 |
| MOTA | 3613 | N | ALA | 518 | 17.272 | 37.965 | 9.988 | 1.00 47.52 |
| MOTA | 3614 | CA | ALA | 518 | 17.379 | 39.358 | 10.404 | 1.00 48.26 |
| ATOM | 3615 | CB | ALA | 518 | 16.748 | 39.540 | 11.780 | 1.00 47.98 |
| MOTA | 3616 | С | ALA | 518 | 18.833 | 39.817 | 10.432 | 1.00 48.77 |
| ATOM | 3617 | 0 | ALA | 518 | 19.113 | 41.014 | . 10.470 | 1.00 48.43 |
| ATOM | 3618 | N | PHE | 519 | 19.758 | 38.863 | 10.412 | 1.00 49.79 |
| ATOM | 3619 | CA | PHE | 519 | 21.178 | 39.193 | 10.437 | 1.00 50.88 |
| ATOM | 3620 | CB | PHE | 519 | 21.810 | 38.675 | 11.723 | 1.00 51.40 |
| ATOM | 3621 | CG | PHE | 519 | 21.076 | 39.092 | 12.957 | 1.00 52.43 |
| | | | | | | | 13.228 | 1.00 52.43 |
| ATOM | 3622 | CD1 | PHE | 519 | 20.855 | 40.436 | | |
| MOTA | 3623 | | PHE | 519 | 20.594 | 38.141 | 13.845 | 1.00 53.65 |
| MOTA | 3624 | | PHE | 519 | 20.160 | 40.829 | 14.369 | 1.00 53.53 |
| ATOM | 3625 | | PHE | 519 | 19.899 | 38.522 | 14.988 | 1.00 54.19 |
| ATOM | 3626 | CZ | PHE | 519 | 19.682 | 39.869 | 15.251 | 1.00 53.89 |
| MOTA | 3627 | С | PHE | 519 | 21.915 | 38.622 | 9.234 | 1.00 51.31 |
| ATOM | 3628 | 0 | PHE | 519 | 23.130 | 38.413 | 9.277 | 1.00 51.70 |
| ATOM | 3629 | N | GLY | 520 | 21.168 | 38.369 | 8.165 | 1.00 51.46 |
| MOTA | 3630 | CA | GLY | 520 | 21.752 | 37.832 | 6.950 | 1.00 52.29 |
| ATOM | 3631 | С | GLY | 520 | 22.668 | 36.646 | 7.172 | 1.00 52.89 |
| ATOM | 3632 | 0 | GLY | 520 | 23.880 | 36.740 | 6.973 | 1.00 52.01 |
| ATOM | 3633 | N | ILE | 521 | 22.085 | 35.526 | 7.582 | 1.00 53.71 |
| ATOM | 3634 | CA | ILE | 521 | 22.844 | 34.309 | 7.830 | 1.00 54.45 |
| ATOM | 3635 | CB | ILE | 521 | 22.669 | 33.839 | 9.287 | 1.00 53.41 |
| | | | | | | 32.580 | 9.531 | 1.00 53.41 |
| ATOM | 3636 | | ILE | 521 | 23.483 | | | |
| MOTA | 3637 | CG1 | ILE | 521 | 23.109 | 34.948 | 10.243 | 1.00 52.97 |
| MOTA | 3638 | CD1 | | 521 | 22.872 | 34.629 | 11.702 | 1.00 51.81 |
| ATOM | 3639 | С | ILE | 521 | 22.375 | 33.201 | 6.894 | 1.00 55.91 |
| MOTA | 3640 | 0 | ILE | 521 | 23.163 | 32.358 | 6.467 | 1.00 56.51 |
| MOTA | 3641 | N | THR | 522 | 21.089 | 33.216 | 6.566 | 1.00 57.60 |
| ATOM | 3642 | CA | THR | 522 | 20.517 | 32.203 | 5.692 | 1.00 60.04 |
| MOTA | 3643 | CB | THR | 522 | 19.147 | 31.738 | 6.218 | 1.00 60.24 |
| ATOM | 3644 | OG1 | THR | 522 | 18.278 | 32.869 | 6.353 | 1.00 59.37 |
| MOTA | 3645 | CG2 | THR | 522 | 19.301 | 31.058 | 7.569 | 1.00 60.73 |
| ATOM | 3646 | C | THR | 522 | 20.355 | 32.683 | 4.252 | 1.00 61.62 |
| ATOM | 3647 | ō | THR | 522 | 19.702 | 33.695 | 3.992 | 1.00 61.80 |
| | - · | - | | | | | | _ |

| ATOM | 3648 | N | GLY | 523 | 20.959 | 31.942 | 3.324 | 1.00 63.15 |
|--------------|--------------|----------|------------|------------|------------------|------------------|--------|--------------------------|
| ATOM | 3649 | CA | GLY | 523 | 20.881 | 32.276 | 1.911 | 1.00 65.08 |
| ATOM | 3650 | С | GLY | 523 | 20.874 | 33.762 | 1.601 | 1.00 66.40 |
| ATOM | 3651 | 0 | GLY | 523 | 21.492 | 34.563 | 2.305 | 1.00 66.60 |
| ATOM | 3652 | N | GLY | 524 | 20.170 | 34.128 | 0.536 | 1.00 66.95 |
| ATOM | 3653 | CA | GLY | 524 | 20.092 | 35.522 | 0.146 | 1.00 67.88 |
| ATOM | 3654 | C | GLY | 524 | 18.666 | 35.958 | -0.116 | 1.00 68.78 |
| ATOM | 3655 | ō | GLY | 524 | 18.280 | 37.078 | 0.220 | 1.00 69.41 |
| ATOM | 3656 | N | HIS | 525 | 17.880 | 35.072 | -0.719 | 1.00 69.01 |
| | 3657 | CA | HIS | 525 | 16.487 | 35.376 | -1.023 | 1.00 69.66 |
| ATOM | | | | | | 34.488 | -2.165 | 1.00 70.70 |
| ATOM | 3658 | CB | HIS | 525 | 15.987 | | -3.520 | 1.00 70.70 |
| ATOM | 3659 | CG | HIS | 525 | 16.435 | 34.939 | -3.520 | |
| ATOM | 3660 | | HIS | 525 | 17.174 | 34.317 | | 1.00 72.56 1.00 72.33 |
| ATOM | 3661 | | HIS | 525 | 16.105 | 36.172 | -4.039 | |
| ATOM | 3662 | | HIS | 525 | 16.620 | 36.290 | -5.250 | 1.00 72.53 |
| ATOM | 3663 | | HIS | 525 | 17.273 | 35.178 | -5.535 | 1.00 72.71 |
| MOTA | 3664 | C | HIS | 525 | 15.578 | 35.208 | 0.191 | 1.00 69.38 |
| MOTA | 3665 | 0 | HIS | 525 | 14.651 | 34.398 | 0.177 | 1.00 69.45 |
| MOTA | 3666 | N | ILE | 526 | 15.849 | 35.979 | 1.240 | 1.00 68.69 |
| MOTA | 3667 | CA | ILE | 526 | 15.047 | 35.922 | 2.457 | 1.00 67.80 |
| MOTA | 3668 | CB | ILE | 526 | 15.558 | 36.927 | 3.512 | 1.00 67.79 |
| MOTA | 3669 | CG2 | ILE | 526 | 17.003 | 36.613 | 3.872 | 1.00 68.10 |
| MOTA | 3670 | CG1 | ILE | 526 | 15.431 | 38.354 | 2.974 | 1.00 67.42 |
| MOTA | 3671 | CD1 | | 526 | 15.759 | 39.424 | 3.991 | 1.00 67.22 |
| MOTA | 3672 | С | ILE | 526 | 13.601 | 36.271 | 2.116 | 1.00 67.09 |
| MOTA | 3673 | 0 | ILE | 526 | 13.325 | 36.817 | 1.050 | 1.00 67.20 |
| MOTA | 3674 | N | PRO | 527 | 12.657 | 35.959 | 3.018 | 1.00 66.11 |
| ATOM | 3675 | CD | PRO | 527 | 12.814 | 35.365 | 4.356 | 1.00 66.02 |
| MOTA | 3676 | CA | PRO | 527 | 11.251 | 36.270 | 2.747 | 1.00 65.35 |
| MOTA | 3677 | CB | PRO | 527 | 10.532 | 35.712 | 3.974 | 1.00 65.35 |
| MOTA | 3678 | CG | PRO | 527 | 11.563 | 35.834 | 5.053 | 1.00 65.87 |
| MOTA | 3679 | С | PRO | 527 | 11.023 | 37.768 | 2.555 | 1.00 64.42 |
| MOTA | 3680 | 0 | PRO | 527 | 11.728 | 38.591 | 3.141 | 1.00 64.06 |
| ATOM | 3681 | N | LYS | 528 | 10.038 | 38.110 | 1.729 | 1.00 63.60 |
| ATOM | 3682 | CA | LYS | 528 | 9.719 | 39.506 | 1.440 | 1.00 62.63 |
| ATOM | 3683 | CB | LYS | 528 | 8.504 | 39.596 | 0.507 | 1.00 63.43 |
| ATOM | 3684 | CG | LYS | 528 | 8.568 | 38.689 | -0.715 | 1.00 64.83 |
| ATOM | 3685 | CD | LYS | 528 | 8.054 | 37.291 | -0.389 | 1.00 65.58 |
| MOTA | 3686 | CE | LYS | 528 | 8.237 | 36.336 | -1.559 | 1.00 65.50 |
| MOTA | 3687 | NZ | LYS | 528 | 9.678 | 36.076 | -1.831 | 1.00 65.11 |
| ATOM | 3688 | C | LYS | 528 | 9.443 | 40.317 | 2.702 | 1.00 61.12 |
| ATOM | 3689 | Ō | LYS | 528 | 9.874 | 41.465 | 2.815 | 1.00 60.81 |
| ATOM | 3690 | N | PHE | 529 | 8.726 | 39.715 | 3.648 | 1.00 59.49 |
| ATOM | 3691 | CA | PHE | 529 | 8.379 | 40.383 | 4.899 | 1.00 57.86 |
| ATOM | 3692 | СВ | PHE | 529 | 7.258 | 39.611 | 5.608 | 1.00 57.20 |
| ATOM | 3693 | CG | PHE | 529 | 7.586 | 38.168 | 5.885 | 1.00 56.39 |
| ATOM | 3694 | | PHE | 529 | 8.487 | 37.820 | 6.887 | 1.00 55.45 |
| ATOM | 3695 | | PHE | 529 | 6.990 | 37.153 | 5.140 | 1.00 56.22 |
| ATOM | 3696 | | PHE | 529 | 8.787 | 36.483 | 7.146 | 1.00 55.50 |
| ATOM | 3697 | CE2 | PHE | 529 | 7.283 | 35.813 | 5.390 | 1.00 55.77 |
| ATOM | 3698 | CZ | PHE | 529 | 8.183 | 35.478 | 6.396 | 1.00 55.99 |
| ATOM | 3699 | C | | 529 | 9.564 | 40.562 | 5.844 | 1.00 56.78 |
| MOTA | 3700 | ō | PHE | 529 | 9.463 | 41.272 | 6.843 | 1.00 56.44 |
| ATOM | 3701 | N | ALA | 530 | 10.684 | 39.923 | 5.525 | 1.00 55.87 |
| ATOM | 3701 | CA | ALA | 530 | 11.878 | 40.015 | 6.357 | 1.00 55.61 |
| ATOM | 3702 | CB | ALA | 530 | 12.612 | 38.681 | 6.366 | 1.00 55.37 |
| ATOM | 3704 | С | ALA | 530 | 12.809 | 41.114 | 5.864 | 1.00 55.36 |
| ATOM | 3705 | o | ALA | 530 | 12.597 | 41.687 | 4.795 | 1.00 55.63 |
| ATOM | 3705 | N | LYS | 531 | 13.842 | 41.399 | 6.651 | 1.00 55.00 |
| ATOM | 3707 | CA | LYS | 531 | 14.816 | 42.425 | 6.301 | 1.00 54.83 |
| ATOM | 3708 | CB | LYS | 531 | 14.303 | 43.806 | 6.712 | 1.00 54.88 |
| ATOM | 3709 | CG | | 531 | 15.283 | 44.932 | 6.428 | 1.00 55.59 |
| | | | LYS | | | | 6.851 | 1.00 55.93 |
| ATOM ATOM | 3710 3711 | CD CE | LYS LYS | 531 531 | 14.726 15.716 | 46.280 47.397 | 6.560 | 1.00 56.02 |
| | | | | | | 48.729 | 6.933 | 1.00 55.93 |
| ATOM | 3712 3713 | NZ | LYS | 531 | | 48.729 | 6.933 | 1.00 54.84 |
| ATOM | 3713 | C | LYS | 531 531 | 16,161 | | 8.154 | 1.00 54.84 |
| ATOM | | O N | LYS | 531 | 16.220 | 41.840 | | |
| MOTA | 3715 | N | ASN | 532 | 17.237 | 42.315 | 6.203 | 1.00 54.78 |
| ATOM | 3716 | CA | ASN | 532 | 18.591 | 42.110 | 6.708 | 1.00 54.97 |
| MOTA | 3717 | CB | ASN | 532 | 19.544 | 41.805 | 5.548 | 1.00 54.87 |
| ATOM | 3718 | CG | ASN | 532 | 20.931 | 41.399 | 6.017 | 1.00 53.96 |
| MOTA | 3719 | | ASN | 532 | 21.469 | 41.963 | 6.970 | 1.00 54.05 |
| MOTA | 3720 | ND2 | | 532 | 21.522 | 40.425 | 5.335 | 1.00 54.07 |
| ATOM | 3721 | C | ASN | 532 | 19.061 | 43.373 | 7.424 | 1.00 55.48 |
| ATOM | 3722 | 0 | ASN | 532 | 19.215 | 44.422 | 6.798 | 1.00 56.16 |
| MOTA | 3723 | N | PHE | 533 | 19.290 | | 8.730 | 1.00 55.65 |
| MOTA | 3724 | CA | PHE | 533 | 19.744 | 44.425 | 9.503 | 1.00 56.07 |
| | | | | | • | | | |

| ATOM | 3725 | СВ | PHE | 533 | 19.055 | 44.463 | 10.871 | 1.00 | 56.06 |
|--------------|--------------|-----------|------------|------------|------------------|------------------|------------------|------|----------------|
| ATOM | 3726 | CG | PHE | 533 | 17.607 | 44.863 | 10.812 | | 56.39 |
| ATOM | 3727 | CD1 | | 533 | 16.649 | 43.993 | 10.303 | 1.00 | 56.26 |
| ATOM | 3728 | CD2 | | 533 | 17.204 | 46.124 | 11.245 | 1.00 | 56.64 |
| MOTA | 3729 | CE1 | PHE | 533 | 15.311 | 44.371 | 10.228 | 1.00 | 56.57 |
| MOTA | 3730 | CE2 | PHE | 533 | 15.868 | 46.511 | 11.173 | 1.00 | 56.36 |
| MOTA | 3731 | CZ | PHE | 533 | 14.921 | 45.634 | 10.663 | 1.00 | 56.79 |
| MOTA | 3732 | С | PHE | 533 | 21.255 | 44.446 | 9.695 | 1.00 | 56.80 |
| MOTA | 3733 | 0 | PHE | 533 | 21.808 | 45.424 | 10.199 | 1.00 | 56.46 |
| MOTA | 3734 | N | LEU | 534 | 21.920 | 43.367 | 9.297 | 1.00 | 57.79 |
| ATOM | 3735 | CA | LEU | 534 | 23.370 | 43.281 | 9.427 | 1.00 | 58.91 |
| MOTA | 3736 | CB | LEU | 534 | 23.811 | 41.820 | 9.535 | 1.00 | 58.06 |
| MOTA | 3737 | CG | LEU | 534 | 25.310 | 41.588 | 9.748 | 1.00 | 57.55 |
| MOTA | 3,738 | CD1 | LEU | 534 | 25.744 | 42.191 | 11.076 | | 56.50 |
| ATOM | 3739 | | LEU | 534 | 25.605 | 40.098 | 9.718 | | 57.05 |
| ATOM | 3740 | С | LEU | 534 | 24.041 | 43.928 | 8.220 | | 60.52 |
| MOTA | 3741 | 0 | LEU | 534 | 25.201 | 44.337 | 8.284 | | 60.29 |
| ATOM | 3742 | N | ALA | 535 | 23.303 | 44.010 | 7.118 | | 62.13 |
| ATOM | 3743 | CA | ALA | 535 | 23.816 | 44.611 | 5.892 | | 64.07 |
| ATOM | 3744 | CB | ALA | 535 | 22.930 | 44.228 | 4.713 | | 64.06 |
| ATOM | 3745 | C . | ALA | 535 | 23.859 | 46.127 | 6.048 | | 65.26 |
| MOTA | 3746 | 0 | ALA | 535 | 24.618 | 46.817 | 5.363 | | 65.11 |
| ATOM | 3747 | N | GLU | 536 | 23.034 | 46.633 | 6.959 | | 66.37 |
| ATOM | 3748 | CA | GLU | 536 | 22.955 | 48.064 | 7.233 7.823 | | 67.19 |
| ATOM | 3749 | CB | GLU | 536 | 21.583 | 48.408 | | | 68.14 |
| ATOM | 3750 | CG | GLU | 536 | 20.397 20.159 | 47.779 | 7.094 | | 69.56 70.40 |
| ATOM | 3751 | CD OE1 | GLU | 536 | | 48.366 | 5.713 4.861 | | 71.10 |
| ATOM | 3752 | | GLU | 536 536 | 21.070 19.053 | 48.290 48.904 | 5.481 | | 70.27 |
| ATOM | 3753 3754 | ·C | GLU GLU | 536 | 24.050 | 48.445 | 8.228 | | 66.96 |
| ATOM ATOM | 3755 | 0 | GLU | 536 | 24.057 | 49.552 | 8.765 | | 67.14 |
| ATOM | 3756 | N | THR | 537 | 24.969 | 47.515 | 8.472 | | 66.36 |
| ATOM | 3757 | CA | THR | 537 | 26.069 | 47.741 | 9.402 | | 65.80 |
| ATOM | 3758 | CB | THR | 537 | 25.557 | 47.783 | 10.860 | | 65.76 |
| ATOM | 3759 | OG1 | THR | 537 | 26.640 | 48.104 | 11.742 | | 65.38 |
| ATOM | 3760 | CG2 | THR | 537 | 24.962 | 46.436 | 11.256 | | 65.93 |
| MOTA | 3761 | C | THR | 537 | 27.121 | 46.637 | 9.269 | | 65.16 |
| ATOM | 3762 | 0 | THR | 537 | 27.200 | 45.962 | 8.242 | | 65.26 |
| ATOM | 3763 | N | GLY | 538 | 27.931 | 46.463 | 10.308 | 1.00 | 64.34 |
| MOTA | 3764 | CA | GLY | 538 | 28.959 | 45.439 | 10.282 | 1.00 | 63.04 |
| ATOM | 3765 | C · | GLY | 538 | 29.062 | 44.734 | 11.617 | 1.00 | 62.37 |
| MOTA | 3766 | 0 | GLY | 538 | 30.023 | 44.011 | 11.883 | 1.00 | 62.04 |
| MOTA | 3767 | N | ASP | 539 | 28.060 | 44.949 | 12.462 | | 61.49 |
| MOTA | 3768 | CA | ASP | 539 | 28.021 | 44.342 | 13.785 | | 60.74 |
| MOTA | 3769 | CB | ASP | 539 | 28.268 | 45.407 | 14.857 | | 62.06 |
| MOTA | 3770 | CG | ASP | 539 | 28.250 | 44.838 | 16.262 | | 63.43 |
| MOTA | 3771 . | | ASP | 539 | 28.222 | 45.633 | 17.226 | | 63.49 |
| ATOM | 3772 | | ASP | 539 | 28.270 | 43.595 | 16.402 | 1.00 | |
| ATOM | 3773 | C | ASP | 539 | 26.666 | 43.684 | 14.023 | | 59.48 |
| ATOM | 3774 | 0 | ASP | 539 | 25.624 | 44.258 | 13.705 | 1.00 | 58.85 |
| ATOM | 3775 | N | ILE | 540 | 26.685 | 42.478 | 14.582 | | 58.12 |
| ATOM | 3776 | CA | ILE | 540 | 25.455 | 41.747 40.355 | 14.867 | | 56.14 57.05 |
| ATOM ATOM | 3777 3778 | CB CG2 | ILE ILE | 540 540 | 25.760 24.458 | 39.622 | 15.456 15.772 | | 56.67 |
| ATOM | 3779 | | ILE | 540 | 26.596 | 39.549 | 14.461 | | 56.82 |
| ATOM | 3780 | | ILE | 540 | 27.153 | 38.264 | 15.030 | | 57.97 |
| ATOM | 3781 | C | ILE | 540 | 24.612 | 42.534 | 15.864 | | 54.58 |
| ATOM | 3782 | 0 | ILE | 540 | 23.410 | 42.714 | 15.669 | | 53.94 |
| ATOM | 3783 | N | ARG | 541 | 25.252 | 43.002 | 16.932 | | 52.23 |
| ATOM | 3784 | CA | ARG | 541 | 24.564 | 43.779 | 17.955 | | 50.98 |
| ATOM | 3785 | CB | ARG | 541 | 25.524 | 44.108 | 19.100 | | 49.65 |
| ATOM | 3786 | CG | ARG | 541 | 26.008 | 42.882 | 19.852 | 1.00 | 48.84 |
| MOTA | 3787 | CD | ARG | 541 | 27.008 | 43.238 | 20.938 | 1.00 | 47.15 |
| ATOM | 3788 | NE | ARG | 541 | 27.476 | 42.053 | 21.655 | 1.00 | 47.04 |
| ATOM | 3789 | CZ | ÁRG | 541 | 28.122 | 41.038 | 21.087 | 1.00 | 47.57 |
| MOTA | 3790 | NH1 | ARG | 541 | 28.383 | 41.054 | 19.787 | | 47.71 |
| MOTA | 3791 | NH2 | ARG | 541 | 28.509 | 40.004 | 21.821 | | 47.56 |
| ATOM | 3792 | С | ARG | 541 | 23.999. | 45.066 | 17.359 | | 50.80 |
| ATOM | 3793 | 0 | ARG | 541 | 22.915 | 45.515 | 17.739 | | 50.76 |
| MOTA | 3794 | N | ALA | 542 | 24.735 | 45.654 | 16.422 | | 50.14 |
| MOTA | 3795 | CA | ALA | 542 | 24.297 | 46.882 | 15.770 | | 49.97 |
| MOTA | 3796 | CB | ALA | 542 | 25.369 | 47.376 | 14.806 | | 49.83 |
| ATOM | 3797 | C | ALA | 542 | 22.996 | 46.614 | | | 49.62 |
| ATOM | 3798 | 0 | ALA | 542 | 22.065 | 47.417 | 15.064 | | 49.97 |
| ATOM | 3799 | N | ALA | 543 | 22.942 | 45.479 | 14.332 | | 49.14 |
| ATOM ATOM | 3800 3801 | CA CB | ALA | 543 543 | 21.753 | 45.095 | 13.583 12.794 | | 48.56 47.62 |
| ATOM | 200I | CB | ALA | 543 | 22.022 | 43.819 | 14.774 | 1.00 | 41.04 |

| ATOM | 3802 | С | ALA | 543 | 20.593 | 44.882 | 14.554 | 1.00 48.49 |
|------|-------|-----|-------|------------------|--------|---------|--------|------------|
| АТОМ | 3803 | O | ALA | 543 | 19.431 | 45.095 | 14.205 | 1.00 48.03 |
| | 3804 | N | VAL | 544 | 20.923 | 44.462 | 15.773 | 1.00 47.91 |
| ATOM | | | | | | | | |
| ATOM | 3805 | CA | VAL | 544 | 19.921 | 44.220 | 16.807 | 1.00 48.15 |
| ATOM | 3806 | CB | VAL | 544 | 20.547 | 43.544 | 18.054 | 1.00 47.72 |
| MOTA | 3807 | CG1 | VAL | 544 | 19.493 | 43.354 | 19.133 | 1.00 48.12 |
| ATOM | 3808 | CG2 | VAL | 544 | 21.151 | 42.203 | 17.670 | 1.00 47.67 |
| ATOM | 3809 | С | VAL | 544 | 19.280 | 45.535 | 17.234 | 1.00 48.25 |
| | 3810 | o | VAL | 544 | 18.055 | 45.670 | 17.229 | 1.00 48.02 |
| MOTA | | | | | | | | |
| MOTA | 3811 | N | ARG | 545. | 20.113 | 46.503 | 17.602 | 1.00 47.95 |
| MOTA | 3812 | CA | ARG | 545 | 19.613 | 47.804 | 18.025 | 1.00 48.51 |
| ATOM | 3813 | СB | ARG | 545 | 20.771 | 48.699 | 18.471 | 1.00 47.82 |
| ATOM | 3814 | CG | ARG | 545 | 21.478 | 48.204 | 19.722 | 1.00 49.07 |
| ATOM | 3815 | CD | ARG | 545 | 22.351 | 49.289 | 20.335 | 1.00 49.84 |
| ATOM | 3816 | NE | ARG | 545 | 23.473 | 49.659 | 19.477 | 1.00 51.11 |
| | | CZ | ARG | 545 | 24.521 | 48.877 | 19.235 | 1.00 51.17 |
| ATOM | 3817 | | | | | | | |
| ATOM | 3818 | | ARG | 545 | 24.596 | 47.674 | 19.787 | 1.00 52.25 |
| ATOM | 3819 | NH2 | ARG | 545 | 25.497 | 49.300 | 18.444 | 1.00 51.42 |
| MOTA | 3820 | C | ARG | 545 | 18.826 | 48.481 | 16.908 | 1.00 48.39 |
| ATOM | 3821 | 0 | ARG | 545 | 17.806 | 49.119 | 17.161 | 1.00 47.66 |
| ATOM | 3822 | N | GLN | 546 | 19.296 | 48.338 | 15.674 | 1.00 49.12 |
| ATOM | 3823 | CA | GLN | 546 | 18.610 | 48.941 | 14.538 | 1.00 50.17 |
| | 3824 | CB | GLN | 546 | 19.428 | 48.766 | 13.257 | 1.00 51.51 |
| MOTA | | | | | | | | |
| ATOM | 3825 | CG | GLN | 546 | 18.835 | 49.481 | 12.052 | 1.00 54.04 |
| ATOM | 3826 | CD | GLN | 546 | 19.635 | 49.256 | 10.786 | 1.00 55.80 |
| MOTA | 3827 | OE1 | GLN | 546 | 20.829 | 49.555 | 10.731 | 1.00 57.97 |
| ATOM | 3828 | NE2 | GLN | 546 | 18.980 | 48.730 | 9.757 | 1.00 56.73 |
| ATOM | 3829 | С | GLN | 546 | 17.245 | 48.282 | 14.369 | 1.00 50.05 |
| ATOM | 3830 | 0 | GLN | 546 | 16.268 | 48.936 | 14.001 | 1.00 49.98 |
| | | | TYR | 547 | 17.189 | 46.982 | 14.640 | 1.00 49.32 |
| MOTA | 3831 | N | | | | | | |
| MOTA | 3832 | CA | TYR | 547 | 15.948 | 46.227 | 14.537 | 1.00 48.54 |
| ATOM | 3833 | СВ | TYR | 547 | 16.203 | 44.750 | 14.840 | 1.00 49.78 |
| ATOM | 3834 | CG | TYR | 547 | 14.944 | 43.925 | 14.955 | 1.00 50.44 |
| MOTA | 3835 | CD1 | TYR | 547 | 14.056 | 43.822 | 13.885 | 1.00 51.69 |
| MOTA | 3836 | CE1 | TYR | 547 | 12.893 | 43.064 | 13.984 | 1.00 51.91 |
| ATOM | 3837 | CD2 | TYR | 547 | 14.637 | 43.249 | 16.135 | 1.00 51.50 |
| ATOM | 3838 | CE2 | | 547 | 13.476 | 42.487 | 16.247 | 1.00 51.56 |
| | | | | | | | 15.168 | 1.00 52.16 |
| ATOM | 3839 | CZ | TYR | 547 | 12.610 | 42.399 | | |
| ATOM | 3840 | OH | TYR | 547 | 11.463 | 41.646 | 15.271 | 1.00 51.53 |
| MOTA | 3841 | С | TYR | 547 | 14.926 | 46.781 | 15.523 | 1.00 47.25 |
| MOTA | 3842 | 0 | TYR | 547 | 13.793 | 47.092 | 15.155 | 1.00 46.01 |
| MOTA | 3843 | N | MET | 548 [′] | 15.345 | 46.902 | 16.779 | 1.00 45.68 |
| ATOM | 3844 | CA | MET | 548 | 14.491 | 47.421 | 17.839 | 1.00 45.05 |
| ATOM | 3845 | CB | MET | 548 | 15.273 | 47.471 | 19.153 | 1.00 43.72 |
| ATOM | 3846 | CG | MET | 548 | 15.852 | 46.136 | 19.574 | 1.00 44.22 |
| | | | | 548 | 17.010 | 46.272 | 20.949 | 1.00 43.86 |
| ATOM | 3847 | SD | MET | | | | | |
| ATOM | 3848 | CE | MET | 548 | 15.902 | 46.115 | 22.333 | 1.00 45.50 |
| MOTA | 3849 | С | MET | 548 | 14.016 | 48.823 | 17.479 | 1.00 45.08 |
| MOTA | 3850 | 0 | MET | 548 | 12.859 | 49.186 | 17.708 | 1.00 43.72 |
| MOTA | 3851 | N | ALA | 549 | 14.929 | 49.603 | 16.910 | 1.00 45.01 |
| ATOM | 3852 | CA | ALA | 549 · | 14.643 | 50.973 | 16.515 | 1.00 45.18 |
| ATOM | 3853 | СВ | ALA | 549 | 15.923 | 51.651 | 16.044 | 1.00 44.23 |
| | 3854 | C | ALA | 549 | 13.581 | 51.042 | 15.424 | 1.00 45.78 |
| ATOM | | | | | | | | 1.00 45.86 |
| ATOM | 3855 | 0 | ALA | 549 | 12.518 | 51.625 | 15.626 | |
| MOTA | 3856 | N | GLU | 550 | 13.867 | 50.442 | 14.272 | 1.00 46.83 |
| ATOM | 3857 | CA | GLU . | 550 | 12.925 | 50.460 | 13.156 | 1.00 48.63 |
| MOTA | 3858 | CB | GLU | 550 | 13.470 | 49.657 | 11.975 | 1.00 49.72 |
| ATOM | 3859 | CG | GLU | 550 | 14.515 | .50.394 | 11.160 | 1.00 51.94 |
| ATOM | 3860 | CD | GLU | 550 | 14.779 | 49.726 | 9.828 | 1.00 53.48 |
| ATOM | 3861 | | GLU | 550 | 13.799 | 49.459 | 9.097 | 1.00 54.23 |
| ATOM | 3862 | | GLU | 550 | 15.961 | 49.474 | 9.506 | 1.00 55.31 |
| | | | | | | | | |
| ATOM | 3863. | C | GLU | 550 | 11.535 | 49.946 | 13.514 | 1.00 49.36 |
| ATOM | 3864 | 0 | GLU | 550 | 10.530 | 50.507 | 13.073 | 1.00 49.22 |
| MOTA | 3865 | N | VAL | 551 | 11.477 | 48.879 | 14.303 | 1.00 48.98 |
| ATOM | 3866 | CA | VAL | 551 | 10.199 | 48.310 | 14.707 | 1.00 49.91 |
| ATOM | 3867 | СВ | VAL | 551 | 10.397 | 47.020 | 15.538 | 1.00 49.52 |
| ATOM | 3868 | | VAL | 551 | 9.066 | 46.544 | 16.094 | 1.00 49.11 |
| ATOM | 3869 | CG2 | | 551 | 11.017 | 45.937 | 14.668 | 1.00 49.69 |
| | | | VAL | 551 | 9.409 | 49.318 | 15.536 | 1.00 50.71 |
| ATOM | 3870 | С | | | | | | |
| ATOM | 3871 | 0 | VAL | 551 | 8.193 | 49.444 | 15.385 | 1.00 50.53 |
| ATOM | 3872 | N | GLU | 552 | 10.110 | 50.036 | 16.408 | 1.00 51.60 |
| MOTA | 3873 | CA | GLU | 552 | 9.481 | 51.032 | 17.264 | 1.00 52.58 |
| MOTA | 3874 | CB | GLU | 552 | 10.379 | 51.324 | 18.468 | 1.00 53.60 |
| ATOM | 3875 | CG | GLU | 552 | 9.753 | 52.241 | 19.503 | 1.00 55.39 |
| ATOM | 3876 | CD | GLU | 552 | 10.650 | 52.453 | 20.704 | 1.00 56.32 |
| MOTA | 3877 | | GLU | 552 | 10.199 | 53.087 | 21.682 | 1.00 56.45 |
| | | | | 552 | 11.808 | 51.987 | 20.670 | 1.00 50.45 |
| MOTA | 3878 | UE2 | GLU | | 11.000 | 21.30/ | 20.070 | 1.00 37.00 |
| | | | | | | | | |

| ATOM | 3879 | С | GLU | 552 | 9.217 | 52.323 | 16.492 | 1.00 53.07 |
|--------------|--------------|---------|------------|-------------|----------------|------------------|----------------|--------------------------|
| ATOM | 3880 | 0 | GLU | 552 | 8.295 | 53.073 | 16.811 | 1.00 52.73 |
| ATOM | 3881 | N | SER | 553 | 10.035 | 52.570 | 15.474 | 1.00 52.74 |
| ATOM | 3882 | CA | SER | 553 | 9.903 | 53.762 | 14.651 | 1.00 53.94 |
| ATOM | 3883 | CB | SER | 553 | 11.230 | 54.065 | 13.956 | 1.00 54.05 |
| MOTA | 3884 | OG | SER | 553 | 12.264 | 54.253 | 14.908 | 1.00 56.04 |
| ATOM | 3885 | С | SER | 553 | 8.811 | 53.583 | 13.603 | 1.00 54.10 |
| ATOM | 3886 | 0 | SER | 553 | 8.314 | 54.556 | 13.034 | 1.00 53.78 |
| ATOM | 3887 | N | GLY | 554 | 8.439 | 52.333 | 13.356 | 1.00 53.73 |
| ATOM | 3888 | CA | GLY | 554 | 7.413 | 52.052 | 12.371 | 1.00 53.14 |
| ATOM | 3889 | С | GLY | 554 | 8.037 | 51.889 | 11.003 | 1.00 53.03 |
| ATOM | 3890 | 0 | GLY | 554 | 7.353 | 51.571 | 10.030 | 1.00 52.59 |
| ATOM | 3891 | N | VAL | 555 | 9.347 | 52.109 | 10.931 | 1.00 52.96 |
| ATOM | 3892 | CA | VAL | 555 | 10.079 | 51.986 | 9.677 | 1.00 52.87 |
| MOTA | 3893 | CB | VAL | 555 | 11.565 | 52.367 | 9.862 | 1.00 53.58 |
| MOTA | 3894 | CG1 | VAL | 555 | 12.285 | 52.329 | 8.523 | 1.00 52.84 |
| ATOM | 3895 | CG2 | VAL | 555 | 11.671 | 53.749 | 10.485 | 1.00 53.08 |
| MOTA | 3896 | С | VAL | 555 | 9.998 | 50.554 | 9.156 | 1.00 52.67 |
| ATOM | 3897 | 0 | VAL | 555 | 9.908 | 50.324 | 7.948 | 1.00 52.23 |
| MOTA | 3898 | N | TYR | 556 | 10.031 | 49.595 | 10.076 | 1.00 52.50 |
| MOTA | 3899 | CA | TYR | 556 | 9.960 | 48.183 | 9.719 | 1.00 51.70 |
| ATOM | 3900 | CB | TYR | 556 | 11.227 | 47.456 | 10.174 | 1.00 51.86 |
| MOTA | 3901 | CG | TYR | 556 | 11.214 | 45.977 | 9.868 | 1.00 51.09 |
| ATOM | 3902 | | TYR | 556 | 11.254 | 45.519 | 8.552 | 1.00 50.94 |
| MOTA | 3903 | | TYR | 556 | 11.189 | 44.160 | 8.260 | 1.00 51.28 |
| MOTA | 3904 | CD2 | TYR | 556 | 11.113 | 45.034 | 10.892 | 1.00 51.14 |
| MOTA | 3905 | CE2 | | 556 | 11.047 | 43.670 | 10.613 | 1.00 50.47 |
| MOTA | 3906 | CZ | TYR | 556 | 11.083 | 43.241 | 9.295 | 1.00 50.81 |
| ATOM | 3907 | OH | TYR | 556 | 10.995 | 41.900 | 9.000 | 1.00 50.30 |
| ATOM | 3908 | C | TYR | 556 | 8.741 | 47.531 | 10.363 | 1.00 51.68 |
| ATOM | 3909 | 0 | TYR | 556 | 8.529 | 47.653 | 11.569 | 1.00 51.15 |
| ATOM | 3910 | N | PRO | 557 | 7.927 | 46.820 | 9.565 | 1.00 52.14 |
| ATOM | 3911 | CD | PRO | 557 | 6.797 | 46.019 | 10.067 | 1.00 52.66 |
| ATOM | 3912 | CA | PRO | 557 | 8.100 | 46.621 | 8.120 | 1.00 52.90 |
| MOTA | 3913 | CB | PRO | -557 | 7.223 | 45.405 | 7.840 | 1.00 52.64 |
| ATOM | 3914 | CG | PRO | 557 | 6.089 | 45.614 | 8.786 | 1.00 52.85 |
| ATOM | 3915 | C | PRO | 557 | 7.684 | 47.839 | 7.292 | 1.00 53.09 |
| ATOM | 3916 | 0 | PRO | 557 | 6.762 | 48.566 | 7.664 | 1.00 53.40 |
| ATOM | 3917 | N | GLY | 558 | 8.366 | 48.050 | 6.170 | 1.00 53.27 |
| ATOM | 3918 | CA | GLY | 558 550 | 8.055 | 49.181 | 5.316 | 1.00 53.66 |
| ATOM | 3919 3920 | С 0 | GLY | 558. 558 | 6.840 5.703 | 48.937 49.072 | 4.444 4.900 | 1.00 54.13 1.00 54.10 |
| MOTA MOTA | 3920 | | GLY | 559 | 7.081 | 49.072 | 3.186 | 1.00 54.10 |
| ATOM | 3922 | N CA | GLU GLU | 559 | 6.001 | 48.309 | 2.245 | 1.00 54.22 |
| ATOM | 3923 | CB | GLU | 559 | 5.822 | 49.482 | 1.276 | 1.00 54.22 |
| ATOM | 3924 | CG | GLU | 559 | 4.536 | 49.415 | 0.461 | 1.00 56.21 |
| ATOM | 3925 | CD | GLU | 559 | 3.295 | 49.590 | 1.321 | 1.00 56.50 |
| ATOM | 3926 | | GLU | 559 | 2.175 | 49.406 | 0.800 | 1.00 57.07 |
| ATOM | 3927 | | GLU | 559 | 3.440 | 49.916 | 2.518 | 1.00 57.08 |
| ATOM | 3928 | C | GLU | 559 | 6.295 | 47.039 | 1.452 | 1.00 54.13 |
| ATOM | 3929 | Ö | GLU | 559 | 5.378 | 46.336 | 1.026 | 1.00 53.98 |
| ATOM | 3930 | N | GLU | 560 | 7.576 | 46.751 | 1.253 | 1.00 53.68 |
| ATOM | 3931 | CA | GLU | 560 | 7.977 | 45.560 | 0.515 | 1.00 54.17 |
| ATOM | 3932 | CB | GLU | 560 | 9.400 | 45.719 | -0.027 | 1.00 54.49 |
| ATOM | 3933 | CG | GLU | 560 | 9.861 | 47.161 | -0.132 | 1.00 55.28 |
| ATOM | 3934 | CD | GLU | 560 | 10.388 | 47.700 | 1.186 | 1.00 55.88 |
| MOTA | 3935 | OE1 | | 560 | 11.523 | 47.335 | 1.563 | 1.00 55.57 |
| ATOM | 3936 | OE2 | GLU | 560 | . 9.668 | 48.478 | 1.850 | 1.00 55.73 |
| MOTA | 3937 | С | GLU | 560 | 7.912 | 44.352 | 1.441 | 1.00 53.99 |
| MOTA | 3938 | 0 | GLU | 560 | 8.119 | 43.215 | 1.014 | 1.00 54.19 |
| ATOM | 3939 | N | HIS | 561 | 7.621 | 44.616 | 2.712 | 1.00 53.66 |
| ATOM | 3940 | CA | HIS | 561 | 7.527 | 43.571 | 3.727 | 1.00 53.03 |
| ATOM | 3941 | CB | HIS | 561 | 8.320 | 43.975 | 4.972 | 1.00 53.33 |
| ATOM | 3942 | CG | HIS | 561 | 9.687 | 44.507 | | 1.00 52.71 |
| MOTA | 3943 | CD2 | | 561 | 10.242 | 45.720 | 4.914 | 1.00 52.67 |
| MOTA | 3944 | ND1 | | 561 | 10.662 | 43.755 | 4.057 | 1.00 52.82 |
| MOTA | 3945 | CE1 | | 561 | 11.758 | 44.482 | 3.926 | 1.00 53.52 |
| MOTA | 3946 | NE2 | | 561 | 11.529 | 45.677 | 4.439 | 1.00 52.58 |
| MOTA | 3947 | ·C | HIS | 561 | 6.073 | 43.340 | 4.124 | 1.00 52.40 |
| ATOM | 3948 | 0 | HIS | 561 | 5.783 | 42.508 | 4.983 | 1.00 52.28 |
| MOTA | 3949 | N | SER | 562 | 5.164 | 44.081 | 3.495 | 1.00 51.41 |
| ATOM | 3950 | CA | SER | 562 | 3.741 | 43.973 | 3.794 | 1.00 50.51 |
| MOTA | 3951 | CB | SER | 562 | 3.172 | 45.359 | 4.106 | 1.00 50.14 |
| ATOM | 3952 | OG | SER | 562 | 3.952 | 46.021 | 5.086 | 1.00 49.54 |
| ATOM | 3953 | С | SER | 562 | 2.956 | 43.350 | 2.644 | 1.00 50.99 |
| MOTA | 3954 | 0 | SER | 562 | 3.381 | 43.398 | 1.488 | 1.00 50.00 |
| ATOM | 3955 | N | PHE | 563 | 1.808 | 42.764 | 2.966 | 1.00 50.96 |

| ATOM | 3956 | CA | PHE | 563 | 0.966 | 42.144 | 1.953 | 1.00 51.90 |
|------|------|-----|----------------|-----|--------|--------|---------|--------------------------|
| ATOM | 3957 | CB | PHE | 563 | 0.792 | 40.649 | 2.230 | 1.00 51.88 |
| ATOM | 3958 | CG | PHE | 563 | 2.085 | 39.889 | 2.291 | 1.00 52.62 |
| ATOM | 3959 | CD1 | | 563 | 2.800 | 39.800 | 3.482 | 1.00 52.62 |
| | 3960 | CD2 | PHE | 563 | 2.598 | 39.274 | 1.154 | 1.00 52.02 |
| ATOM | | | | | | | | |
| ATOM | 3961 | CE1 | PHE | 563 | 4.008 | 39.107 | 3.540 | 1.00 53.30 |
| ATOM | 3962 | CE2 | PHE | 563 | 3.805 | 38.580 | 1.200 | 1.00 53.30 |
| ATOM | 3963 | CZ | PHE | 563 | 4.512 | 38.496 | 2.397 | 1.00 53.09 |
| ATOM | 3964 | С | PHE | 563 | -0.396 | 42.820 | 1.925 | 1.00 52.18 |
| ATOM | 3965 | . 0 | PHE | 563 | -0.847 | 43.371 | 2.930 | 1.00 51.96 |
| ATOM | 3966 | N | HIS | 564 | -1.051 | 42.775 | 0.771 | 1.00 53.34 |
| MOTA | 3967 | CA | HIS | 564 | -2.362 | 43.394 | 0.617 | 1.00 54.06 |
| MOTA | 3968 | CB | HIS | 564 | -2.228 | 44.709 | -0.155 | 1.00 54.83 |
| MOTA | 3969 | CG | HIS | 564 | -1.305 | 45.696 | 0.493 | 1.00 55.50 |
| ATOM | 3970 | | HIS | 564 | -0.118 | 46.206 | 0.086 | 1.00 55.30 |
| ATOM | 3971 | | HIS | 564 | -1.564 | 46.262 | 1.722 | 1.00 55.51 |
| MOTA | 3972 | | HIS | 564 | -0.577 | 47.079 | 2.046 | 1.00 55.52 |
| ATOM | 3973 | | HIS | 564 | 0.314 | 47.062 | 1.070 | 1.00 55.47 |
| ATOM | 3974 | C | HIS | 564 | -3.315 | 42.457 | -0.111 | 1.00 54.29 |
| ATOM | 3975 | 0 | HIS | 564 | -4.385 | 42.152 | 0.454 | 1.00 54.03 |
| | 3976 | | | | | | -1.238 | |
| ATOM | | | HIS | 564 | -2.978 | 42.040 | | 1.00 55.99 |
| ATOM | 3977 | C1 | KPL | 565 | 8.381 | 32.905 | 12.296 | 1.00 41.48 |
| MOTA | 3978 | C2 | KPL | 565 | 7.795 | 33.008 | 13.719 | 1.00 41.70 |
| MOTA | 3979 | C3 | KPL | 565 | 8.747 | 33.842 | 14.588 | 1.00 41.04 |
| MOTA | 3980 | C4 | KPL | 565 | 6.432 | 33.729 | 13.657 | 1.00 42.99 |
| ATOM | 3981 | 01 | \mathtt{KPL} | 565 | 5.502 | 32.994 | 12.852 | 1.00 47.23 |
| MOTA | 3982 | C5 | \mathtt{KPL} | 565 | 7.641 | 31.587 | 14.333 | 1.00 41.12 |
| MOTA | 3983 | 02 | KPL | 565 | 6.548 | 31.189 | 14.686 | 1.00 40.23 |
| MOTA | 3984 | C6 | KPL | 565 | 8.827 | 30.664 | 14.510 | 1.00 39.79 |
| ATOM | 3985 | 03 | KPL | 565 | 9.940 | 31.012 | 14.179 | 1.00 41.42 |
| ATOM | 3986 | 04 | KPL | 565 | 8.649 | 29.440 | 15.040 | 1.00 37.97 |
| MOTA | 3987 | CB | MET | 601 | 10.230 | | -10.646 | 1.00 69.60 |
| ATOM | 3988 | CG | MET | 601 | 9.281 | | -11.531 | 1.00 71.50 |
| ATOM | 3989 | SD | MET | 601 | 7.632 | | -11.738 | 1.00 73.80 |
| | 3990 | CE | | 601 | 6.646 | | -10.716 | 1.00 73.00 |
| ATOM | | | MET | | | | | |
| ATOM | 3991 | C | MET | 601 | 8.842 | 22.547 | -9.089 | 1.00 66.93 |
| ATOM | 3992 | 0 | MET | 601 | 8.861 | 23.439 | -9.940 | 1.00 67.03 |
| MOTA | 3993 | N | MET | 601 | 9.123 | 20.086 | -8.698 | 1.00 68.90 |
| ATOM | 3994 | CA | MET | 601 | 9.767 | 21.337 | -9.196 | 1.00 68.18 |
| ATOM | 3995 | N | LYS | 602 | 8.036 | 22.570 | -8.032 | 1.00 64.76 |
| ATOM | 3996 | CA | LYS | 602 | 7.110 | 23.667 | -7.796 | 1.00 62.08 |
| MOTA | 3997 | CB | LYS | 602 | 5.693 | 23.272 | -8.237 | 1.00 63.38 |
| MOTA | 3998 | CG | LYS | 602 | 5.557 | 23.006 | -9.732 | 1.00 64.55 |
| MOTA | 3999 | CD | LYS | 602 | 5.683 | 24.288 | -10.545 | 1.00 65.81 |
| MOTA | 4000 | CE | LYS | 602 | 4.492 | 25.207 | -10.311 | 1.00 65.96 |
| ATOM | 4001 | NZ | LYS | 602 | 4.629 | 26.497 | -11.038 | 1.00 66.71 |
| ATOM | 4002 | С | LYS | 602 | 7.105 | 24.081 | -6.322 | 1.00 59.15 |
| ATOM | 4003 | O | LYS | 602 | 7.250 | 25.263 | -6.006 | 1.00 59.60 |
| ATOM | 4004 | N | PRO | 603 | 6.959 | 23.112 | -5.396 | 1.00 55.04 |
| ATOM | 4005 | CD | PRO | 603 | 7.155 | 23.394 | -3.964 | 1.00 54.14 |
| ATOM | 4006 | CA | PRO | 603 | 6.772 | 21.673 | -5.613 | 1.00 51.11 |
| | 4007 | | PRO | | | 21.075 | | |
| ATOM | | CB | | 603 | 7.269 | | -4.303 | 1.00 52.30 1.00 53.08 |
| ATOM | 4008 | CG | PRO | 603 | 6.782 | 22.075 | -3.311 | |
| MOTA | 4009 | C | PRO | 603 | 5.317 | 21.318 | -5.889 | 1.00 46.82 |
| ATOM | 4010 | 0 | PRO | 603 | 4.426 | 22.143 | -5.704 | 1.00 47.26 |
| | 4011 | N | THR | 604 | 5.079 | 20.088 | -6.329 | 1.00 41.84 |
| ATOM | 4012 | CA | THR | 604 | 3.727 | 19.639 | -6.627 | 1.00 36.41 |
| ATOM | 4013 | CB | THR | 604 | 3.742 | 18.241 | -7.268 | 1.00 36.28 |
| MOTA | 4014 | OG1 | THR | 604 | 4.564 | 18.265 | -8.440 | 1.00 34.78 |
| MOTA | 4015 | CG2 | THR | 604 | 2.331 | 17.811 | -7.650 | 1.00 35.28 |
| ATOM | 4016 | C | THR | 604 | 2.902 | 19.582 | -5.350 | 1.00 33.25 |
| ATOM | 4017 | 0 | THR | 604 | 3.270 | 18.893 | -4.398 | 1.00 31.12 |
| MOTA | 4018 | N | THR | 605 | 1.792 | 20.314 | -5.326 | 1.00 30.68 |
| ATOM | 4019 | CA | THR | 605 | 0.929 | 20.327 | -4.153 | 1.00 29.21 |
| ATOM | 4020 | CB | THR | 605 | 0.921 | 21.708 | -3.465 | 1.00 29.89 |
| ATOM | 4021 | OG1 | THR | 605 | 0.134 | 22.625 | -4.236 | 1.00 30.44 |
| ATOM | 4022 | | THR | 605 | 2.341 | 22.245 | -3.336 | 1.00 29.99 |
| ATOM | 4023 | C | THR | 605 | -0.505 | 19.970 | -4.524 | 1.00 27.07 |
| | | | | | | | -5.700 | |
| MOTA | 4024 | 0 | THR | 605 | -0.823 | 19.779 | | 1.00 25.26 |
| MOTA | 4025 | N | ILE | 606 | -1.358 | 19.885 | -3.508 | 1.00 24.97 |
| ATOM | 4026 | CA | ILE | 606 | -2.767 | 19.551 | -3.684 | 1.00 24.26 |
| ATOM | 4027 | CB | ILE | 606 | -3.495 | 19.497 | -2.318 | 1.00 26.83 |
| ATOM | 4028 | CG2 | ILE | 606 | -4.942 | 19.052 | -2.510 | 1.00 24.52 |
| MOTA | 4029 | CG1 | ILE | 606 | -2.767 | 18.531 | -1.381 | 1.00 28.76 |
| MOTA | 4030 | CD1 | ILE | 606 | -3.204 | 18.634 | 0.077 | 1.00 32.70 |
| MOTA | 4031 | С | ILE | 606 | -3.459 | 20.593 | -4.558 | 1.00 22.72 |
| | 402T | - | | | | | | |
| MOTA | 4031 | Ō | ILE | 606 | -4.297 | 20.259 | -5.397 | 1.00 21.59 |

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ATOM
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             OE2 GLU
                        615
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| ATOM | 4110 | С | GLU | 615 | -9.277 | 20.707 | -17.115 | 1.00 16.72 |
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| ATOM | 4111 | 0 | GLU | 615 | -9.025 | 20.543 | -18.310 | 1.00 16.29 |
| ATOM | 4112 | N | LYS | 616 | -9.869 | 19.778 | -16.371 | 1.00 17.52 |
| ATOM | 4113 | CA | LYS | 616 | -10.210 | 18.460 | -16.915 | 1.00 20.17 |
| ATOM | 4114 | CB | LYS | 616 | -11.254 | 18.567 | -18.027 | 1.00 23.07 |
| MOTA | 4115 | CG | LYS | 616 | -12.604 | 19.120 | -17.606 | 1.00 29.30 |
| MOTA | 4116 | CD | LYS | 616 | -13.410 | 18.131 | -16.789 | 1.00 32.57 |
| MOTA | 4117 | CE | LYS | 616 | -14.817 | 18.660 | -16.536 | 1.00 33.31 |
| MOTA | 4118 | NZ | LYS | 616 | -15.508 | | -17.807 | 1.00 38.09 |
| MOTA | 4119 | С | LYS | 616 | -8.950 | | -17.475 | 1.00 21.00 |
| MOTA | 4120 | 0 | LYS | 616 | -8.993 | | -18.455 | 1.00 21.94 |
| ATOM | 4121 | N | LYS | 617 | -7.818 | | -16.864 | 1.00 18.27 |
| MOTA | 4122 | CA | LYS | 617 | -6.557 | | -17.298 | 1.00 17.56 |
| ATOM | 4123 | CB | LYS | 617 | -5.427 | | -17.183 | 1.00 20.70 |
| MOTA | 4124 | CG | LYS | 617 | -4.111 | | -17.736 | 1.00 23.47 |
| MOTA | 4125 | CD | LYS | 617 | -2.959 | | -17.311 | 1.00 27.46 |
| ATOM | 4126 | CE | LYS | 617 | -3.104 | | -17.847 | 1.00 28.51 |
| ATOM | 4127 | NZ | LYS | 617 | -2.146 | | -17.160 | 1.00 31.20 |
| MOTA | 4128 | C | LYS | 617 | -6.266 | | -16.399 | 1.00 16.64 |
| MOTA | 4129 | 0 | LYS | 617 | -5.821 | | -15.263 | 1.00 14.57 |
| MOTA | 4130 | N | ARG | 618 | -6.536 | | -16.910 -16.149 | 1.00 16.67 1.00 14.83 |
| MOTA | 4131 4132 | CA CB | ARG ARG | 618 618 | -6.320 - 6.910 | | -16.149 | 1.00 14.83 |
| MOTA MOTA | 4133 | CG | ARG | 618 | -8.434 | | -16.882 | 1.00 13.02 |
| ATOM | 4134 | CD | ARG | 618 | -9.058 | | -17.852 | 1.00 23.21 |
| ATOM | 4135 | NE | ARG | 618 | -8.928 | | -19.232 | 1.00 25.21 |
| ATOM | 4136 | CZ | ARG | 618 | -9.601 | | -20.258 | 1.00 20.23 |
| ATOM | 4137 | NH1 | | 618 | -10.458 | | -20.060 | 1.00 27.55 |
| ATOM | 4138 | | ARG | 618 | -9.421 | | -21.480 | 1.00 25.20 |
| ATOM | 4139 | С | ARG | 618 | -4.838 | | -15.865 | 1.00 15.48 |
| ATOM | 4140 | ō | ARG | 618 | -3.999 | | -16.748 | 1.00 16.70 |
| ATOM | 4141 | N | PHE | 619 | -4.519 | | -14.619 | 1.00 14.70 |
| ATOM | 4142 | CA | PHE | 619 | -3.131 | | -14.213 | 1.00 13.63 |
| ATOM | 4143 | CB | PHE | 619 | -2.797 | 14.341 | -13.158 | 1.00 14.26 |
| MOTA | 4144 | CG | PHE | 619 | -3.688 | 14.296 | -11.951 | 1.00 15.87 |
| ATOM | 4145 | CD1 | PHE | 619 | -3.411 | 13.431 | -10.894 | 1.00 14.85 |
| MOTA | 4146 | CD2 | PHE | 619 | -4.816 | 15.109 | -11.875 | 1.00 17.83 |
| ATOM | 4147 | CE1 | PHE - | 619 | -4.244 | 13.374 | -9.778 | 1.00 14.51 |
| MOTA | 4148 | CE2 | PHE | 619 | -5.657 | | -10.764 | 1.00 17.27 |
| MOTA | 4149 | CZ | PHE | 619 . | -5.370 | 14.191 | -9.711 | 1.00 15.64 |
| MOTA | 4150 | С | PHE | 619 | -2.815 | | -13.671 | 1.00 15.10 |
| MOTA | 4151 | 0 | PHE | 619 | -3.660 | | -13.051 | 1.00 14.55 |
| ATOM | 4152 | N | ALA | 620 | -1.586 | | -13.903 | 1.00 13.79 |
| ATOM. | 4153 | CA | ALA | 620 | -1.144 | | -13.440 | 1.00 14.57 |
| ATOM | 4154 | CB | ALA | 620 | -0.186 | | -14.460 | 1.00 14.31 |
| ATOM | 4155 4156 | С | ALA | 620 620 | -0.482 0.149 | | -12.067 -11.687 | 1.00 14.58 1.00 13.79 |
| ATOM ATOM | 4157 | N O | ALA THR | 621 | -0.646 | | -11.322 | 1.00 13.79 |
| ATOM | 4158 | CA | THR | 621 | -0.073 | 8.962 | -9.994 | 1.00 12.67 |
| ATOM | 4159 | | THR | 621 | -1.145 | 9.145 | -8.912 | 1.00 14.02 |
| ATOM | 4160 | OG1 | | 621 | -1.660 | 10.482 | -8.982 | 1.00 22.56 |
| ATOM | 4161 | CG2 | THR | 621 | -0.567 | 8.893 | -7.550 | 1.00 25.02 |
| ATOM | 4162 | C | THR | 621 | 0.457 | 7.538 | -9.925 | 1.00 13.44 |
| ATOM | 4163 | o ` | THR | 621 | -0.023 | | -10.643 | 1.00 13.17 |
| MOTA | 4164 | N | ILE | 622 | 1.428 | 7.296 | -9.059 | 1.00 14.11 |
| ATOM | 4165 | CA | ILE | 622 | 1.984 | 5.958 | -8.979 | 1.00 14.52 |
| ATOM | 4166 | CB | ILE | 622 | 3.165 | 5.825 | -9. 9 85 | 1.00 16.11 |
| ATOM | 4167 | CG2 | ILE | 622 | 4.372 | 6.630 | -9.495 | 1.00 19.85 |
| ATOM | 4168 | CG1 | ILE | 622 | 3.500 | | -10.204 | 1.00 19.83 |
| MOTA | 4169 | CD1 | ILE | 622 | 4.468 | | -11.347 | 1.00 22.61 |
| ATOM | 4170 | C | ILE | 622 | 2.443 | 5.606 | -7.570 | 1.00 13.66 |
| MOTA | 4171 | 0 | ILE | 622 | 2.596 | 6.481 | -6.735 | 1.00 12.92 |
| ATOM | 4172 | N | THR | 623 | 2.611 | 4.317 | -7.295 | 1.00 15.34 |
| ATOM | 4173 | CA | THR | 623 | 3.080 | 3.914 | -5.979 | 1.00 16.08 |
| ATOM. | 4174 | CB | THR | 623 | 2.611 | 2.491 | -5.595 | 1.00 16.42 |
| ATOM | 4175 | OG1 | THR | 623 | 3.187 | 1.540 | -6.498 | 1.00 19.41 |
| ATOM | 4176 | | THR | 623 | 1.090 | 2.390 | -5.656 -6.063 | 1.00 19.47 |
| ATOM | 4177 | C | THR | 623 | 4.602 | 3.910 | -6.063 | 1.00 14.73 |
| MOTA | 4178 | O N | THR | 623 | 5.162 | 3.799 4.030 | -7.150 -4.913 | 1.00 14.80 1.00 14.62 |
| MOTA | 4179 4180 | N | ALA ALA | 624 624 | 5.260 6.719 | 4.030 | -4.913 -4.826 | 1.00 14.62 |
| ATOM ATOM | 4180 | CA CB | ALA | 624 | 7.282 | 5.398 | -5.187 | 1.00 14.03 |
| MOTA | 4182 | СВ | ALA | 624 | 7.081 | 3.680 | -3.384 | 1.00 13.13 |
| ATOM | 4183 | 0 | ALA | 624 | 6.417 | 4.135 | -2.452 | 1.00 14.07 |
| MOTA | 4184 | N | TYR | 625 | 8.126 | 2.885 | -3.186 | 1.00 14.04 |
| ATOM | 4185 | CA | TYR | 625 | 8.504 | 2.522 | -1.830 | 1.00 13.33 |
| ATOM | 4186 | CB . | TYR | 625 | 7.992 | 1.125 | -1.478 | 1.00 13.65 |
| _ | | | - | | | • | | |

| ATOM | 4187 | CG | TYR | 625 | 6.658 | 0.790 | -2.089 | 1.00 11.16 |
|--------------|--------------|-----------|------------|------------|----------------|--------|--------------------|--------------------------|
| ATOM | 4188 | CD1 | | 625 | 6.587 | 0.065 | -3.277 | 1.00 13.08 |
| ATOM | 4189 | CE1 | | 625 | 5.367 | -0.253 | -3.852 | 1.00 12.70 |
| ATOM | 4190 | CD2 | TYR | 625 | 5.467 | 1.199 | -1.488 | 1.00 11.45 |
| ATOM | 4191 | CE2 | TYR | 625 | 4.234 | 0.886 | -2.057 | 1.00 11.45 |
| ATOM | 4192 | CZ | TYR | 625 | 4.194 | 0.155 | -3.241 | 1.00 11.70 |
| ATOM | 4193 | ОН | TYR | 625 | 2.993 | -0.200 | -3.795 | 1.00 13.12 |
| MOTA | 4194 | С | TYR | 625 | 9.999 | 2.555 | -1.624 | 1.00 14.79 |
| ATOM | 4195 | 0 | TYR | 625 | 10.500 | 2.009 | -0.640 | 1.00 12.38 |
| ATOM | 4196 | N | ASP | 626 | 10.721 | 3.177 | -2.549 | 1.00 14.45 |
| ATOM | 4197 | CA | ASP | 626 | 12.166 | 3.263 | -2.410 | 1.00 16.17 |
| ATOM | 4198 | CB | ASP | 626 | 12.837 | 1.949 | -2.862 | 1.00 18.23 |
| MOTA | 4199 | CG | ASP | 626 | 12.721 | 1.703 | -4.362 | 1.00 19.53 |
| ATOM | 4200 | | ASP | 626 | 13.387 | 2.419 | -5.136 | 1.00 19.59 |
| ATOM | 4201 | | ASP | 626 | 11.964 | 0.792 | -4.764 | 1.00 21.03 |
| ATOM | 4202 | С | ASP | 626 | 12.746 | 4.454 | -3.159 | 1.00 16.01 |
| MOTA | 4203 | 0 | ASP | 626 | 12.091 | 5.068 | -4.009 | 1.00 15.86 |
| ATOM | 4204 | N | TYR | 627 | 13.989 | 4.771 | -2.826 | 1.00 15.06 |
| ATOM | 4205 | CA | TYR | 627 | 14.695 | 5.896 | -3.419 | 1.00 15.15 |
| ATOM | 4206 | CB | TYR | 627 | 16.058 | 6.039 | -2.745 | 1.00 16.61 |
| ATOM | 4207 | CG | TYR | 627 | 16.991 | 7.003 | -3.440 | 1.00 17.55 |
| ATOM | 4208 | CD1 | TYR | 627 | 17.025 | 8.351 | -3.089 | 1.00 17.88 |
| MOTA | 4209 | CE1 | TYR | 627 | 17.901 | 9.237 | -3.714 | 1.00 18.86 |
| MOTA | 4210 | CD2 | TYR | 627. | 17.854 | 6.561 | -4.441 | 1.00 18.63 |
| MOTA | 4211 | CE2 | TYR | 627 | 18.728 | 7.435 | -5.073 | 1.00 20.28 |
| ATOM | 4212 | cz | TYR | 627 | 18.746 | 8.763 | -4.703 | 1.00 21.00 |
| ATOM | 4213 | ОН | TYR | 627 | 19.624 | 9.615 | -5.330 | 1.00 23.89 |
| MOTA | 4214 | C | TYR | 627 · | 14.892 | 5.816 | -4.929 | 1.00 15.66 |
| ATOM | 4215 | 0 | TYR | 627 | 14.681 | 6.797 | -5.635 | 1.00 15.39 |
| MOTA | 4216 | N | SER | 628 | 15.300 | 4.653 | -5.422 | 1.00 15.60 |
| MOTA | 4217 | CA | SER | 628 | 15.568 | 4.504 | -6.842 | 1.00 16.14 |
| ATOM | 4218 | CB | SER | 628 | 16.196 | 3.139 | -7.111 | 1.00 16.61 |
| MOTA | 4219 | OG | SER | 628 | 17.466 | 3.068 | -6.473 | 1.00 18.25 |
| MOTA | 4220 | C | SER | 628 | 14.367 | 4.733 | -7.746 | 1.00 16.64 |
| ATOM | 4221 | 0 | SER | 628 | 14.448 | 5.505 | -8.702 | 1.00 14.62 |
| ATOM | 4222 | N | PHE | 629 | 13.249 | 4.081 | -7.462 | 1.00 16.10 |
| MOTA | 4223 | CA | PHE | 629 | 12.090 | 4.303 | -8.307 | 1.00 15.35 |
| MOTA | 4224 | CB | PHE | 629 | 11.032 | 3.225 | -8.069 | 1.00 15.85 |
| ATOM | 4225 | CG | PHE | 629 | 11.350 | 1.934 | -8.769 | 1.00 16.27 |
| MOTA | 4226 | CD1 | PHE | 629 | 12.022 | 0.910 | -8.108 | 1.00 15.67 |
| MOTA | 4227 | CD2 | PHE | 629 | 11.039 | 1.774 | -10.118 | 1.00 14.97 |
| MOTA | 4228 | CE1 | PHE | 629 | 12.381 | -0.261 | -8.781 | 1.00 16.45 |
| MOTA | 4229 | | PHE | 629 | 11.391 | | -10.803 | 1.00 15.51 |
| MOTA | 4230 | cz | PHE | 629 | 12.066 | | -10.137 | 1.00 15.52 |
| MOTA | 4231 | С | PHE | 629 | 11.526 | | | |
| MOTA | 4232 | 0 | PHE | 629 | 11.149 | 6.362 | -9.110 | 1.00 14.31 |
| MOTA | 4233 | N | ALA | 630 | 11.509 | 6.210 | -6.900 | 1.00 13.96 |
| MOTA | 4234 | CA | ALA | 630 | 10.998 | 7.554 | -6.654 | 1.00 13.58 |
| ATOM | 4235 | CB | ALA | 630 | 11.058 | 7.872 | -5.164 | 1.00 15.22 |
| MOTA | 4236 | C | ALA | 630 | 11.800 | 8.585 | -7.447 | 1.00 14.75 |
| MOTA | 4237 | 0 | ALA | 630 | 11.240 | 9.526 | -8.024 | 1.00 14.71 |
| MOTA | 4238 | | LYS | | 13.115 | 8.408 | -7.467 | 1.00 15.76 |
| ATOM | 4239 | CA | LYS | 631 | 14.011 | 9.312 | -8.193 | 1.00 17.34 |
| ATOM | 4240 | CB | LYS | 631 | 15.465 | 8.898 | | 1.00 17.65 |
| MOTA | 4241 | CG . | LYS | 631 | 16.529 | 9.653 | -8.706 | 1.00 23.27 |
| ATOM | 4242 | CD | LYS | 631 | 16.611 | 11.105 | -8.294 | 1.00 24.41 |
| ATOM | 4243 | CE | LYS | 631 | 17.957 | 11.707 | -8.699 | 1.00 28.34 |
| ATOM | 4244 | NZ | LYS | 631 | 18.224 | | -10.164 | 1.00 29.72 |
| ATOM | 4245 | C | LYS | 631 | 13.703 | 9.244 | -9.689 | 1.00 16.69 |
| ATOM | 4246 | 0 | LYS | 631 | 13.628 | | -10.375 | 1.00 17.77 |
| MOTA | 4247 | N | LEU | 632 | 13.527 | | -10.193 | 1.00 15.74 |
| ATOM | 4248 | CA | LEU | 632 | 13.224 | | -11.606 | 1.00 14.84 |
| MOTA | 4249 | CB | LEU | 632 | 13.153 | | -11.916 | 1.00 15.29 |
| ATOM | 4250 | CG | LEU | 632 | 13.100 | | -13.390 | 1.00 14.76 |
| ATOM | 4251 | | LEU | 632 | 13.590 | | -13.492 | 1.00 13.45 |
| ATOM | 4252 4253 | | LEU | 632 | 11.689 | | -13.954 -11.997 | 1.00 14.18 1.00 16.72 |
| ATOM | | С | LEU | 632 | 11.909 | | | |
| ATOM | 4254 | O N | LEU | 632 | 11.834 | | -13.035 -11.177 | 1.00 15.36 |
| ATOM | 4255 | N | PHE | 633 | 10.872 | | -11.177 | 1.00 15.97 1.00 17.44 |
| ATOM | 4256 | CA | PHE | 633 | 9.581 | | -11.477 -10.493 | 1.00 17.44 |
| ATOM | 4257 | CB | PHE | 633 " | 8.497 8.333 | | -10.493 | 1.00 16.12 |
| ATOM | 4258 | CG CD1 | PHE. | 633 | 8.333 | | -10.425 | 1.00 17.21 |
| ATOM | 4259 4260 | | PHE | 633 | 7.921 | 6.350 | -9.240 | 1.00 18.33 |
| ATOM | 4260 4261 | | PHE | 633 | 7.921 8.386 | | -11.483 | 1.00 18.31 |
| ATOM ATOM | 4261 | | PHE PHE | 633 633 | 7.739 | | -9.167 | 1.00 17.33 |
| ATOM | 4263 | CZ | PHE | 633 | 7.974 | | -10.291 | 1.00 14.03 |
| ALOH | 4400 | C4 | EHE | 000 | 1.2/4 | 4.11 | AV.491 | |

| ATOM | 4264 | C | PHE | 633 | 9.683 | 10.464 | -11.409 | 1.00 19.16 |
|------|------|-------|----------------------|-----|--------|--------|---------|------------|
| ATOM | 4265 | 0 | PHE | 633 | 9.128 | 11.173 | -12.251 | 1.00 20.23 |
| ATOM | 4266 | N | ALA | 634 | 10.390 | 10.964 | -10.402 | 1.00 18.95 |
| ATOM | 4267 | CA | ALA | 634 | 10.561 | | -10.235 | 1.00 20.80 |
| MOTA | 4268 | СВ | ALA | 634 | 11.315 | 12.697 | -8.941 | 1.00 22.92 |
| ATOM | 4269 | C | ALA | 634 | 11.314 | | -11.423 | 1.00 21.47 |
| | | | | | | | | 1.00 21.47 |
| MOTA | 4270 | 0 | ALA | 634 | 10.970 | - | -11.903 | |
| ATOM | 4271 | N | ASP | 635 | 12.339 | | -11.898 | 1.00 21.14 |
| MOTA | 4272 | CA | ASP | 635 | 13.113 | | -13.030 | 1.00 23.15 |
| MOTA | 4273 | CB | ASP | 635 | 14.366 | | -13.249 | 1.00 24.84 |
| MOTA | 4274 | CG | ASP | 635 | 15.388 | 12.102 | -12.141 | 1.00 24.40 |
| MOTA | 4275 | OD1 | ASP | 635 | 15.242 | 13.015 | -11.300 | 1.00 27.97 |
| MOTA | 4276 | . OD2 | ASP | 635 | 16.349 | 11.311 | -12.127 | 1.00 26.01 |
| ATOM | 4277 | С | ASP | 635 | 12.319 | 12.844 | -14.338 | 1.00 23.85 |
| ATOM | 4278 | 0 | ASP | 635 | 12.662 | 13.606 | -15.247 | 1.00 23.95 |
| ATOM | 4279 | N | GLU | 636 | 11.269 | | -14.434 | 1.00 22.21 |
| ATOM | 4280 | CA | GLU | 636 | 10.432 | | -15.629 | 1.00 22.88 |
| ATOM | 4281 | CB | GLU | 636 | 9.971 | | -15.899 | 1.00 22.80 |
| | | | | | | | -16.233 | 1.00 22.00 |
| ATOM | 4282 | CG | GLU | 636 | 11.087 | | | |
| ATOM | 4283 | CD | GLU | 636 | 11.863 | | -17.459 | 1.00 25.48 |
| MOTA | 4284 | | GLU | 636 | 11.236 | | -18.523 | 1.00 28.84 |
| MOTA | 4285 | OE2 | | 636 | 13.092 | | -17.359 | 1.00 26.19 |
| MOTA | 4286 | С | GLU | 636 | 9.203 | | -15.543 | 1.00 21.66 |
| MOTA | 4287 | 0 | GLU | 636 | 8.483 | 13.035 | -16.528 | 1.00 22.31 |
| MOTA | 4288 | N | GLY | 637 | 8.939 | 13.435 | -14.365 | 1.00 20.53 |
| ATOM | 4289 | CA | GLY | 637 | 7.789 | 14.308 | -14.223 | 1.00 20.79 |
| ATOM | 4290 | С | GLY | 637 | 6.590 | 13.755 | -13.472 | 1.00 21.60 |
| ATOM | 4291 | Ō | GLY | 637 | 5.582 | | -13.348 | 1.00 22.27 |
| ATOM | 4292 | N | LEU | 638 | 6.680 | | -13.000 | 1.00 21.20 |
| ATOM | 4293 | CA | LEU | 638 | 5.599 | | -12.228 | 1.00 22.21 |
| | 4294 | | | 638 | 5.683 | | -12.301 | 1.00 22.21 |
| ATOM | | CB | LEU | | | | | |
| MOTA | 4295 | CG | LEU | 638 | 4.426 | | -12.774 | 1.00 26.98 |
| MOTA | 4296 | | LEU | 638 | 4.678 | 8.133 | -12.758 | 1.00 25.19 |
| MOTA | 4297 | | LEU | 638 | 3.241 | | -11.903 | 1.00 27.34 |
| MOTA | 4298 | С | LEU | 638 | 5.876 | | -10.807 | 1.00 20.11 |
| MOTA | 4299 | Ο. | LEU | 638 | 6.683 | 11.752 | -10.094 | 1.00 22.26 |
| ATOM | 4300 | N | ASN | 639 | 5.203 | 13.427 | -10.409 | 1.00 20.38 |
| MOTA | 4301 | CA | ASN | 639 | 5.415 | 14.035 | -9.105 | 1.00 18.91 |
| MOTA | 4302 | CB | ASN | 639 | 5.557 | 15.555 | -9.264 | 1.00 24.25 |
| ATOM | 4303 | CG | ASN | 639 | 6.571 | 15.944 | -10.327 | 1.00 28.84 |
| ATOM | 4304 | | ASN | 639 | 7.684 | | -10.361 | 1.00 31.74 |
| MOTA | 4305 | ND2 | | 639 | 6.195 | | -11.194 | 1.00 31.59 |
| ATOM | 4306 | C | ASN | 639 | 4.348 | 13.747 | -8.054 | 1.00 17.68 |
| | | | | | | | | 1.00 17.00 |
| ATOM | 4307 | 0 | ASN | 639 | 4.240 | 14.470 | -7.061 | |
| ATOM | 4308 | N | VAL | 640 | 3.547 | 12.711 | -8.265 | 1.00 16.43 |
| ATOM | 4309 | CA | VAL | 640 | 2.518 | 12.366 | -7.289 | 1.00 15.98 |
| ATOM | 4310 | CB | VAL | 640 | 1.101 | 12.590 | -7.840 | 1.00 16.39 |
| MOTA | 4311 | CG1 | VAL | 640 | 0.083 | 12.203 | -6.787 | 1.00 18.52 |
| MOTA | 4312 | CG2 | VAL | 640 | 0.917 | 14.054 | -8.224 | 1.00 18.53 |
| MOTA | 4313 | C | VAL | 640 | 2.712 | 10.895 | -6.973 | 1.00 15.29 |
| ATOM | 4314 | 0 | VAL | 640 | 2.445 | 10.036 | -7.811 | 1.00 11.74 |
| ATOM | 4315 | N | MET | 641 | 3.190 | 10.618 | -5.764 | 1.00 13.95 |
| ATOM | 4316 | CA | MET | 641 | 3.477 | 9.252 | -5.362 | 1.00 14.10 |
| MOTA | 4317 | CB | MET | 641 | 4.989 | 9.052 | -5.237 | 1.00 14.03 |
| ATOM | 4318 | CG | MET | 641 | 5.725 | 9.242 | -6.546 | 1.00 18.23 |
| ATOM | 4319 | SD | MET | 641 | 7.481 | 9.167 | -6.340 | 1.00 18.97 |
| | 4319 | CE | MET | 641 | 8.019 | 10.537 | -7.397 | 1.00 20.65 |
| ATOM | | | | | 2.815 | 8.827 | -4.076 | 1.00 20.03 |
| MOTA | 4321 | C | MET | 641 | | 9.599 | | |
| MOTA | 4322 | 0 | MET | 641 | 2.704 | | -3.127 | 1.00 16.15 |
| ATOM | 4323 | N | LEU | 642 | 2.405 | 7.569 | -4.041 | 1.00 13.58 |
| ATOM | 4324 | CA | LEU | 642 | 1.743 | 7.045 | -2.865 | 1.00 15.28 |
| MOTA | 4325 | CB | LEU | 642 | 0.330 | 6.602 | -3.257 | 1.00 19.13 |
| ATOM | 4326 | CG | LEU | 642 | -0.652 | 5.954 | -2.276 | 1.00 23.45 |
| ATOM | 4327 | CD1 | LEU | 642 | -0.395 | 4.474 | -2.248 | 1.00 25.41 |
| ATOM | 4328 | | LEU | 642 | -0.555 | 6.576 | -0.881 | 1.00 22.82 |
| ATOM | 4329 | Ċ | LEU | 642 | 2.533 | 5.908 | -2.230 | 1.00 15.23 |
| ATOM | 4330 | ō | LEU | 642 | 2.920 | 4.947 | -2.898 | 1.00 15.25 |
| ATOM | 4331 | N | VAL | 643 | 2.782 | 6.053 | -0.933 | 1.00 16.09 |
| ATOM | 4332 | CA | VAL | 643 | 3.478 | 5.037 | -0.155 | 1.00 16.71 |
| ATOM | 4332 | CB | VAL | 643 | 4.389 | 5.668 | 0.917 | 1.00 15.71 |
| | | | | | 5.181 | 4.576 | 1.632 | 1.00 13.03 |
| MOTA | 4334 | | VAL | 643 | | | | |
| ATOM | 4335 | CG2 | | 643 | 5.351 | 6.663 | 0.261 | 1.00 20.05 |
| ATOM | 4336 | С | VAL | 643 | 2.327 | 4.297 | 0.508 | 1.00 15.14 |
| MOTA | 4337 | 0 | VAL | 643 | 1.931 | 4.624 | 1.624 | 1.00 15.03 |
| ATOM | 4338 | N | GLY | 644 | 1.784 | 3.313 | -0.206 | 1.00 18.13 |
| ATOM | 4339 | CA | GLY | 644 | 0.646 | 2.565 | 0.288 | 1.00 16.80 |
| ATOM | 4340 | С | GLY | 644 | 0.948 | 1.249 | 0.963 | 1.00 16.33 |
| | | | | | | | | |

| ATOM | 4341 | 0 | GLY | 644 | 2.038 | 0.698 | 0.802 | 1.00 15.86 |
|--------|------|-----|-----|-----|--------|---------|--------|------------|
| ATOM | 4342 | N | ASP | 645 | -0.020 | 0.735 | 1.717 | 1.00 15.60 |
| ATOM | 4343 | CA | ASP | 645 | 0.200 | -0.529 | 2.411 | 1.00 16.74 |
| ATOM | 4344 | CB | ASP | 645 | -0.837 | -0.755 | 3.521 | 1.00 15.16 |
| ATOM | 4345 | CG | ASP | 645 | -2.268 | -0.790 | 3.017 | 1.00 16.47 |
| | | OD1 | | 645 | ~2.499 | -0.772 | 1.794 | 1.00 10.47 |
| ATOM | 4346 | | | | | | | |
| MOTA | 4347 | OD2 | | 645 | -3.178 | -0.843 | 3.875 | |
| MOTA | 4348 | C | ASP | 645 | 0.258 | -1.703 | 1.446 | 1.00 15.61 |
| ATOM | 4349 | 0 | ASP | 645 | 0.406 | -2.856 | 1.860 | 1.00 18.52 |
| ATOM | 4350 | N | SER | 646 | 0.169 | -1.399 | 0.151 | 1.00 14.45 |
| ATOM | 4351 | CA | SER | 646 | 0.283 | -2.425 | -0.879 | 1.00 12.93 |
| ATOM | 4352 | CB | SER | 646 | 0.062 | -1.821 | -2.266 | 1.00 14.70 |
| ATOM | 4353 | OG | SER | 646 | 0.943 | -0.726 | -2.478 | 1.00 16.74 |
| ATOM | 4354 | С | SER | 646 | 1.695 | -2.994 | -0.801 | 1.00 13.99 |
| ATOM | 4355 | 0 | SER | 646 | 1.969 | -4.085 | -1.308 | 1.00 15.91 |
| ATOM | 4356 | N | LEU | 647 | 2.596 | -2.248 | -0.170 | 1.00 11.90 |
| ATOM | 4357 | CA | LEU | 647 | 3.977 | -2.702 | -0.031 | 1.00 12.24 |
| ATOM | 4358 | CB | LEU | 647 | 4.839 | -1.599 | 0.601 | 1.00 12.62 |
| | | | | | 4.542 | -1.162 | 2.038 | 1.00 12.02 |
| ATOM | 4359 | CG | LEU | 647 | | | | |
| ATOM | 4360 | CD1 | | 647 | 5.201 | -2.120 | 3.026 | 1.00 15.69 |
| ATOM | 4361 | CD2 | | 647 | 5.062 | 0.254 | 2.247 | 1.00 14.93 |
| MOTA | 4362 | С | LEU | 647 | 4.015 | -3.975 | 0.818 | 1.00 12.53 |
| MOTA | 4363 | 0 | LEU | 647 | 4.983 | -4.728 | 0.765 | 1.00 13.66 |
| ATOM _ | 4364 | N | GLY | 648 | 2.954 | -4.216 | 1.586 | 1.00 12.76 |
| MOTA | 4365 | CA | GLY | 648 | 2.910 | -5.410 | 2.417 | 1.00 12.76 |
| MOTA | 4366 | С | GLY | 648 | 2.941 | -6.654 | 1.554 | 1.00 13.52 |
| ATOM | 4367 | 0 | GLY | 648 | 3.395 | -7.720 | 1.973 | 1.00 12.64 |
| ATOM | 4368 | N | MET | 649 | 2.456 | -6.510 | 0.328 | 1.00 13.40 |
| ATOM | 4369 | CA | MET | 649 | 2.434 | -7.615 | -0.611 | 1.00 13.82 |
| MOTA | 4370 | CB | MET | 649 | 1.068 | -7.672 | -1.307 | 1.00 15.15 |
| | | CG | MET | 649 | -0.080 | -7.870 | -0.326 | 1.00 19.61 |
| ATOM | 4371 | | | | | | | |
| ATOM | 4372 | SD | MET | 649 | -1.749 | -7.781 | -1.021 | 1.00 23.07 |
| ATOM | 4373 | CE | MET | 649 | -1.676 | -9.060 | -2.275 | 1.00 19.40 |
| MOTA | 4374 | C | MET | 649 | 3.563 | -7.497 | -1.631 | 1.00 14.32 |
| MOTA | 4375 | 0 | MET | 649 | 4.352 | -8.418 | -1.802 | 1.00 13.75 |
| MOTA | 4376 | N | THR | 650 | 3.678 | -6.353 | -2.290 | 1.00 12.15 |
| ATOM | 4377 | CA | THR | 650 | 4.717 | -6.216 | -3.303 | 1.00 13.72 |
| ATOM | 4378 | CB | THR | 650 | 4.416 | -5.015 | -4.221 | 1.00 15.77 |
| ATOM | 4379 | OG1 | THR | 650 | 4.506 | -3.803 | -3.475 | 1.00 21.01 |
| ATOM | 4380 | CG2 | THR | 650 | 3.011 | -5.143 | -4.785 | 1.00 15.50 |
| ATOM | 4381 | С | THR | 650 | 6.144 | -6.135 | -2.776 | 1.00 12.32 |
| ATOM | 4382 | ō | THR | 650 | 7.089 | -6.565 | -3.445 | 1.00 11.07 |
| ATOM | | N | VAL | 651 | 6.310 | -5.595 | -1.576 | 1.00 11.07 |
| | 4383 | | | | | | | |
| ATOM | 4384 | CA | VAL | 651 | 7.645 | -5.477 | -0.995 | 1.00 12.05 |
| ATOM | 4385 | CB | VAL | 651 | 7.845 | -4.079 | -0.358 | 1.00 12.18 |
| MOTA | 4386 | | VAL | 651 | 9.211 | -3.993 | 0.316 | 1.00 13.43 |
| MOTA | 4387 | | VAL | 651 | 7.711 | -3.005 | -1.423 | 1.00 13.62 |
| MOTA | 4388 | С | VAL | 651 | 7.895 | -6.557 | 0.057 | 1.00 11.83 |
| MOTA | 4389 | О | VAL | 651 | 8.858 | -7.316 | -0.035 | 1.00 12.12 |
| MOTA | 4390 | N | GLN | 652 | 7.018 | -6.640 | 1.049 | 1.00 12.39 |
| ATOM · | 4391 | CA | GLN | 652 | 7.204 | -7.615 | 2.123 | 1.00 13.70 |
| ATOM | 4392 | CB | GLN | 652 | 6.420 | -7.177 | 3.350 | 1.00 13.40 |
| ATOM | 4393 | CG | GLN | 652 | 6.796 | -5.783 | 3.818 | 1.00 13.66 |
| ATOM | 4394 | CD | GLN | 652 | 6.004 | -5.362 | 5.028 | 1.00 13.82 |
| ATOM | 4395 | | GLN | 652 | 4.978 | -5.962 | 5.340 | 1.00 14.37 |
| ATOM | 4396 | NE2 | | 652 | 6.464 | -4.319 | 5.713 | 1.00 9.59 |
| | | | | | 6.845 | -9.053 | 1.770 | 1.00 13.88 |
| ATOM | 4397 | C | GLN | 652 | | | | |
| ATOM | 4398 | 0 | GLN | 652 | 7.356 | -9.982 | 2.388 | 1.00 14.21 |
| ATOM | 4399 | N | GLY | 653 | 5.957 | -9.239 | 0.799 | 1.00 12.48 |
| ATOM | 4400 | CA | GLY | 653 | 5.595 | -10.590 | 0.408 | 1.00 14.75 |
| ATOM | 4401 | С | GLY | 653 | | -11.249 | 1.193 | 1.00 14.96 |
| ATOM | 4402 | 0 | GLY | 653 | 4.323 | -12.468 | 1.144 | 1.00 14.96 |
| ATOM | 4403 | N | HIS | 654 | 3.693 | -10.461 | 1.924 | 1.00 14.70 |
| ATOM | 4404 | CA | HIS | 654 | 2.572 | -11.008 | 2.678 | 1.00 18.41 |
| ATOM | 4405 | CB | HIS | 654 | 2.150 | -10.052 | 3.792 | 1.00 15.90 |
| ATOM | 4406 | CG | HIS | 654 | 3.191 | -9.857 | 4.844 | 1.00 17.16 |
| ATOM | 4407 | | HIS | 654 | 3.830 | -8.740 | 5.265 | 1.00 12.42 |
| ATOM | 4408 | | HIS | 654 | 3.677 | -10.892 | 5.614 | 1.00 12.42 |
| | | | | | 4.571 | -10.692 | 6.463 | |
| ATOM | 4409 | | HIS | 654 | | | | 1.00 17.70 |
| ATOM | 4410 | | HIS | 654 | 4.683 | -9.118 | 6.272 | 1.00 15.36 |
| MOTA | 4411 | С | HIS | 654 | 1.387 | | 1.745 | 1.00 18.82 |
| ATOM | 4412 | 0 | HIS | 654 | 1.349 | -10.723 | 0.631 | 1.00 20.21 |
| MOTA | 4413 | N | ASP | 655 | | -12.034 | 2.216 | 1.00 19.49 |
| MOTA | 4414 | CA | ASP | 655 | | -12.374 | 1.436 | 1.00 20.72 |
| MOTA | 4415 | CB | ASP | 655 | -1.406 | -13.663 | 1.978 | 1.00 25.65 |
| MOTA | 4416 | CG | ASP | 655 | -2.228 | -13.426 | 3.234 | 1.00 28.75 |
| MOTA | 4417 | | ASP | 655 | -3.324 | -12.830 | 3.133 | 1.00 36.14 |
| | | | | | | | | |

| ATOM | 4418 | OD2 | ASP | 655 | -1.789 | -13.825 | 4.330 | 1.00 34.78 |
|---------|-------|-----|-------|------|--------|---------|---------|------------|
| ATOM | 4419 | С | ASP | 655 | 1 015 | -11.263 | 1.458 | 1.00 19.20 |
| | | | | | | | | |
| MOTA | 4420 | 0 | ASP | 655 | -2.805 | -11.320 | 0.729 | 1.00 20.52 |
| ATOM | 4421 | N | SER | 656 | -1.610 | -10.267 | 2.310 | 1.00 16.01 |
| | | | | | | | | |
| MOTA | 4422 | CA | SER | 656 | -2.545 | -9.149 | 2.407 | 1.00 14.62 |
| ATOM | 4423 | CB | SER | 656 | -3.663 | -9.467 | 3.402 | 1.00 14.60 |
| ATOM | 4424 | OG | SER | 656 | -3.203 | -9.327 | 4.731 | 1.00 13.62 |
| | | | | | | | | |
| ATOM | 4425 | С | SER | 656 | -1.771 | -7.940 | 2.897 | 1.00 11.97 |
| ATOM | 4426 | 0 | SER | 656 | -0.579 | -8.031 | 3.185 | 1.00 11.43 |
| | | | | | | | | |
| MOTA | 4427 | N | THR | 657 | -2.447 | -6.801 | 2.993 | 1.00 13.16 |
| ATOM | 4428 | CA | THR | 657 | -1.801 | -5.578 | 3.461 | 1.00 12.70 |
| ATOM | 4429 | CB | THR | 657 | -2.433 | -4.325 | 2.799 | 1.00 14.37 |
| | | | | | | | | |
| ATOM | 4430 | OGI | THR | 657 | -3.782 | -4.183 | 3.240 | 1.00 14.29 |
| ATOM | 4431 | CG2 | THR | 657 | -2.421 | -4.441 | 1.279 | 1.00 16.57 |
| ATOM | 4432 | С | THR | 657 | -1.852 | -5.394 | 4.980 | 1.00 12.71 |
| | | | | | | | | |
| MOTA | 4433 | 0 | THR | 657 | -1.148 | -4.550 | 5.519 | 1.00 13.29 |
| ATOM | 4434 | N | LEU | 658 | -2.675 | -6.177 | 5.675 | 1.00 14.03 |
| | | CA | | 658 | -2.823 | -6.012 | 7.135 | 1.00 13.77 |
| MOTA | 4435 | | LEU | | | | | |
| ATOM | 4436 | CB | LEU | 658 | -3.780 | -7.076 | 7.692 | 1.00 15.46 |
| MOTA | 4437 | CG | LEU | 658 | -5.279 | -6.806 | 7.474 | 1.00 17.50 |
| | | | | | | | | |
| ATOM | 4438 | | LEU | 658 | ~5.634 | -7.040 | 6.012 | 1.00 21.01 |
| MOTA | 4439 | CD2 | LEU | 658 | -6.099 | -7.729 | 8.372 | 1.00 18.31 |
| MOTA | 4440 | С | LEU | 658 | -1.561 | -5.951 | 8.003 | 1.00 12.69 |
| | | | | | | | | |
| MOTA | 4441 | 0 | LEU | 658 | -1.485 | -5.150 | 8.927 | |
| ATOM | 4442 | N | PRO | 659 | -0.558 | -6.799 | 7.722 | 1.00 14.97 |
| ATOM | 4443 | CD | PRO | 659 | -0.581 | -7.923 | 6.772 | 1.00 12.48 |
| | | | | | | | | |
| MOTA | 4444 | CA | PRO | 659 | 0.685 | -6.810 | 8.501 | 1.00 12.86 |
| ATOM | 4445 | CB | PRO | 659 | 1.425 | -8.038 | 7.957 | 1.00 14.97 |
| ATOM | 4446 | CG | . PRO | 659 | 0.870 | -8.175 | 6.570 | 1.00 21.34 |
| | | | | | | | | |
| ATOM | 4447 | С | PRO | 659 | 1.540 | -5.546 | 8.448 | 1.00 13.36 |
| MOTA | 4448 | 0 | PRO | 659 | 2.434 | -5.365 | 9.273 | 1.00 14.03 |
| ATOM | 4449 | N | VAL | 660 | 1.271 | -4.668 | 7.487 | 1.00 13.75 |
| | | | | | | | | |
| MOTA | 4450 | CA | VAL | 660 | 2.031 | -3.427 | 7.358 | 1.00 12.32 |
| MOTA | 4451 | CB | VAL | 660 | 1.619 | -2.672 | 6.069 | 1.00 12.31 |
| | | | VAL | 660 | 2.316 | -1.318 | 5.990 | 1.00 13.70 |
| MOTA | 4452 | | | | | | | |
| MOTA | 4453 | CG2 | VAL | 660 | 1.962 | -3.515 | 4.868 | 1.00 10.14 |
| MOTA | 4454 | С | VAL | 660 | 1.794 | -2.536 | 8.563 | 1.00 13.42 |
| | | | | | | | | |
| ATOM | 4455 | 0 | | -660 | 0.649 | -2.261 | 8.936 | 1.00 14.34 |
| ATOM | 4456 | N | THR | 661 | 2.878 | -2.077 | 9.176 | 1.00 11.86 |
| ATOM | 4457 | CA | THR | 661 | 2.772 | -1.221 | 10.357 | 1.00 15.36 |
| | | | | | | | | |
| ATOM | -4458 | CB | THR | 661 | 3.795 | -1.640 | 11.439 | 1.00 17.87 |
| MOTA | 4459 | OG1 | THR | 661 | 3.640 | -3.039 | 11.736 | 1.00 21.53 |
| ATOM | 4460 | CG2 | THR | 661 | 3.569 | -0.835 | 12.720 | 1.00 22.77 |
| | | | | | | | | |
| ATOM | 4461 | C | THR | 661 | 3.051 | 0.233 | 9.998 | 1.00 14.14 |
| ATOM · | 4462 | 0 | THR | 661 | 3.553 | 0.517 | - 8.916 | 1.00 11.93 |
| ATOM | 4463 | N | VAL | 662 | 2.722 | 1.141 | 10.912 | 1.00 13.31 |
| | | | | | | | | |
| MOTA | 4464 | CA | VAL | 662 | 2.969 | 2.560 | 10.712 | 1.00 15.63 |
| ATOM | 4465 | CB | VAL | 662 | 2.465 | 3.395 | 11.912 | 1.00 15.72 |
| ATOM | 4466 | CG1 | | 662 | 3.002 | 4.809 | 11.832 | 1.00 18.60 |
| | | | | | | | | |
| MOTA | 4467 | CG2 | VAL | 662 | 0.938 | 3.412 | 11.921 | 1.00 15.56 |
| ATOM | 4468 | C | VAL | 662 | 4.471 | 2.758 | 10.556 | 1.00 15.26 |
| MOTA | 4469 | 0 | VAL | 662 | 4.913 | 3.566 | 9.740 | 1.00 15.83 |
| | | | | | | | | |
| MOTA | 4470 | N | ALA | 663 | 5.255 | 2.004 | 11.323 | 1.00 14.05 |
| ATOM | 4471 | CA | ALA | 663 | 6.707 | 2.100 | 11.236 | 1.00 14.62 |
| ATOM | 4472 | CB | ALA | 663 | 7.364 | 1.189 | 12.278 | 1.00 15.71 |
| | | | | | | | | |
| ATOM | 4473 | C | ALA | 663 | 7.178 | 1.733 | 9.830 | 1.00 14.13 |
| ATOM | 4474 | 0 | ALA | 663 | 8.092 | 2.370 | 9.302 | 1.00 13.75 |
| ATOM . | 4475 | N | ASP | 664 | 6.556 | 0.729 | 9.210 | 1.00 14.22 |
| | | | | | | | | |
| MOTA | 4476 | CA | ASP | 664 | 6.966 | 0.354 | 7.849 | 1.00 13.17 |
| MOTA | 4477 | CB | ASP | 664 | 6.232 | -0.886 | 7.327 | 1.00 13.69 |
| ATOM | 4478 | CG | ASP | 664 | 6.434 | -2.115 | 8.200 | 1.00 11.91 |
| | | | | | | | | |
| MOTA | 4479 | OD1 | | 664 | 7.525 | -2.275 | 8.780 | 1.00 10.98 |
| MOTA | 4480 | OD2 | ASP | 664 | 5.494 | -2.925 | 8.257 | 1.00 14.69 |
| ATOM | 4481 | С | ASP | 664 | 6.650 | 1.494 | 6.895 | 1.00 12.45 |
| | | | | | | | | |
| MOTA | 4482 | 0 | ASP | 664 | 7.472 | 1.838 | 6.047 | 1.00 10.45 |
| MOTA | 4483 | N | ILE | 665 | 5.454 | 2.067 | 7.015 | 1.00 11.31 |
| ATOM | 4484 | CA | ILE | 665 | 5.088 | 3.165 | 6.126 | 1.00 11.92 |
| | | | | | | | | |
| ATOM | 4485 | CB | ILE | 665 | 3.680 | 3.717 | 6.429 | 1.00 13.42 |
| ATOM | 4486 | CG2 | ILE | 665 | 3.406 | 4.942 | 5.556 | 1.00 14.44 |
| ATOM | 4487 | CG1 | ILE | 665 | 2.621 | 2.645 | 6.162 | 1.00 11.06 |
| | | | | | | | | |
| ATOM | 4488 | CD1 | ILE | 665 | 2.482 | 2.252 | 4.704 | 1.00 14.31 |
| MOTA | 4489 | С | ILE | 665 | 6.097 | 4.299 | 6.243 | 1.00 12.95 |
| MOTA | 4490 | 0 | ILE | 665 | 6.547 | 4.845 | 5.227 | 1.00 12.47 |
| | | | | | | | | |
| MOTA | 4491 | N | ALA | 666 | 6.453 | 4.643 | 7.481 | 1.00 13.58 |
| ATOM | 4402 | CA | ALA | 666 | 7.406 | 5.725 | 7.764 | 1.00 13.36 |
| 211 011 | 4492 | ~ | | | | | | |
| ATOM | 4493 | СВ | ALA | 666 | 7.528 | 5.929 | 9.275 | 1.00 13.24 |

4494 C

666

8.788 5.468

7.167 1.00 13.44

| ATOM | 4495 | 0 | ALA | 666 | 9.435 | 6.386 | 6.656 | 1.00 11.50 |
|------|------|------|-----|------------|----------|---------|--------|------------|
| MOTA | 4496 | N | TYR | 667 | 9.232 | 4.215 | 7.242 | 1.00 12.26 |
| ATOM | 4497 | CA | TYR | 667 | 10.528 | 3.806 | 6.703 | 1.00 12.09 |
| | 4498 | CB | TYR | 667 | 10.760 | 2.315 | 6.987 | 1.00 12.31 |
| ATOM | 4499 | CG | TYR | 667 | 12.002 | 1.719 | 6.345 | 1.00 12.31 |
| ATOM | | | | | | | | 1.00 11.83 |
| ATOM | 4500 | CD1 | TYR | 667 | 13.277 | 1.995 | 6.845 | |
| ATOM | 4501 | CE1 | TYR | 667 | 14.418 | 1.421 | 6.275 | 1.00 14.36 |
| ATOM | 4502 | CD2 | TYR | 667 | 11.897 | 0.855 | 5.252 | 1.00 15.01 |
| MOTA | 4503 | CE2 | TYR | 667 | 13.027 | 0.280 | 4.673 | 1.00 13.37 |
| MOTA | 4504 | CZ | TYR | 667 | 14.286 | 0.568 | 5.189 | 1.00 15.02 |
| ATOM | 4505 | ОН | TYR | 667 | 15.404 | 0.011 | 4.612 | 1.00 14.89 |
| ATOM | 4506 | С | TYR | 667 | 10.556 | 4.050 | 5.194 | 1.00 11.94 |
| ATOM | 4507 | 0 | TYR | 667 | 11.453 | 4.712 | 4.672 | 1.00 9.26 |
| ATOM | 4508 | N | HIS | 668 | 9.565 | 3.501 | 4.499 | 1.00 12.01 |
| ATOM | 4509 | CA | HIS | 668 | 9.473 | 3.670 | 3.057 | 1.00 13.41 |
| ATOM | 4510 | CB | HIS | 668 | 8.423 | 2.713 | 2.486 | 1.00 12.37 |
| ATOM | 4511 | CG | HIS | 668 | 8.849 | 1.278 | 2.536 | 1.00 11.83 |
| ATOM | 4512 | | HIS | 668 | 8.557 | 0.293 | 3.419 | 1.00 11.45 |
| | | | HIS | 668 | 9.774 | 0.746 | 1.663 | 1.00 13.13 |
| ATOM | 4513 | | | | | | | 1.00 13.13 |
| ATOM | 4514 | | HIS | 668 | 10.038 | -0.503 | 2.008 | |
| MOTA | 4515 | | HIS | 668 | 9.312 | -0.801 | 3.071 | 1.00 11.79 |
| MOTA | 4516 | С | HIS | 668 | 9.159 | 5.117 | 2.682 | 1.00 14.60 |
| ATOM | 4517 | 0 | HIS | 668 | 9.641 | 5.618 | 1.662 | 1.00 16.39 |
| ATOM | 4518 | N | THR | 669 | 8.369 | 5.803 | 3.501 | 1.00 15.65 |
| MOTA | 4519 | CA | THR | 669 | 8.042 | 7.197 | 3.202 | 1.00 16.31 |
| ATOM | 4520 | CB | THR | 669 | 7.070 | 7.797 | 4.250 | 1.00 15.04 |
| MOTA | 4521 | OG1 | THR | 669 | 5.787 | 7.170 | 4.110 | 1.00 15.98 |
| ATOM | 4522 | CG2 | THR | 669 | 6.914 | 9.314 | 4.036 | 1.00 15.38 |
| MOTA | 4523 | С | THR | 669 | 9.313 | 8.046 | 3.133 | 1.00 15.41 |
| ATOM | 4524 | 0 | THR | 669 | 9.495 | .8.841 | 2.202 | 1.00 15.01 |
| ATOM | 4525 | N | ALA | 670 | 10.205 | 7.858 | 4.104 | 1.00 15.82 |
| ATOM | 4526 | CA | ALA | 670 | 11.458 | 8.615 | 4.151 | 1.00 14.91 |
| | 4527 | CB | ALA | 670 | 12.230 | 8.272 | 5.426 | 1.00 16.01 |
| ATOM | | | | | 12.333 | 8.349 | , | 1.00 16.01 |
| ATOM | 4528 | C | ALA | 670 | | | | |
| ATOM | 4529 | 0 | ALA | 670 | 13.005 | 9.255 | 2.416 | 1.00 14.84 |
| MOTA | 4530 | N | ALA | 671 | 12.337 | 7.098 | 2.483 | 1.00 15.41 |
| MOTA | 4531 | CA | ALA | 671 | 13.141 | 6.713 | 1.327 | 1.00 15.41 |
| ATOM | 4532 | CB | ALA | 671 | 13.162 | 5.184 | 1.190 | 1.00 14.87 |
| MOTA | 4533 | С | ALA | 671 | 12.606 | 7.359 | 0.049 | 1.00 16.10 |
| ATOM | 4534 | 0 13 | ALA | 671 | 13.377 | 7.832 | -0.794 | 1.00 14.32 |
| ATOM | 4535 | N | VAL | 672 | 11.285 | 7.382 | -0.096 | 1.00 14.00 |
| MOTA | 4536 | CA | VAL | 672 | 10.677 | 8.000 | -1.269 | 1.00 14.46 |
| ATOM | 4537 | CB | VAL | 672 | 9.148 | 7.738 | -1.313 | 1.00 15.01 |
| ATOM | 4538 | CG1 | VAL | 672 | 8.482 | 8.651 | -2.351 | 1.00 15.50 |
| ATOM | 4539 | | VAL | 672 | 8.891 | 6.278 | -1.686 | 1.00 16.48 |
| ATOM | 4540 | C | VAL | 672 | 10.933 | 9.508 | -1.270 | 1.00 14.16 |
| ATOM | 4541 | ō | VAL | 672 | 11.181 | 10.108 | -2.322 | 1.00 15.05 |
| ATOM | 4542 | N | ARG | 673 | 10.883 | 10.125 | -0.095 | 1.00 13.51 |
| | | CA | | | 11.109 | | | 1.00 15.06 |
| ATOM | 4543 | | ARG | 673 | | | | 1.00 15.00 |
| MOTA | 4544 | CB | ARG | 673 | 10.777 | 12.086 | 1.390 | |
| MOTA | 4545 | CG | ARG | 673 | 11.038 | 13.580 | 1.570 | 1.00 16.26 |
| MOTA | 4546 | CD | | 673 | 10.302 | 14.412 | 0.532 | 1.00 15.12 |
| MOTA | 4547 | NE | ARG | 673 | 8.877 | 14.529 | 0.829 | 1.00 16.62 |
| ATOM | 4548 | CZ | ARG | 673 | 7.983 | 15.058 | 0.001 | 1.00 17.11 |
| MOTA | 4549 | NH1 | | 673 | 8.361 | 15.518 | -1.187 | 1.00 16.70 |
| MOTA | 4550 | NH2 | ARG | 673 | 6.712 | 15.137 | 0.361. | 1.00 15.79 |
| MOTA | 4551 | С | ARG | 673 | 12.535 | 11.937 | -0.384 | 1.00 16.05 |
| ATOM | 4552 | 0 | ARG | 673 | 12.764 | 12.998 | -0.963 | 1.00 16.70 |
| MOTA | 4553 | N | ARG | 674 | 13.490 | 11.072 | -0.050 | 1.00 15.93 |
| MOTA | 4554 | CA | ARG | 674 | 14.883 | 11.332 | -0.394 | 1.00 17.55 |
| ATOM | 4555 | CB | ARG | 674 | 15.814 | 10.311 | 0.279 | 1.00 17.79 |
| ATOM | 4556 | CG | ARG | 674 | 15.769 | .10.334 | 1.806 | 1.00 17.42 |
| ATOM | 4557 | CD | ARG | 674 | 16.944 | 9.589 | 2.437 | 1.00 19.60 |
| ATOM | 4558 | NE | ARG | 674 | 16.811 | 9.507 | 3.894 | 1.00 22.66 |
| ATOM | 4559 | CZ | ARG | 674 | 16.242 | 8.494 | 4.544 | 1.00 22.60 |
| ATOM | 4559 | NH1 | | | 15.755 | | 3.874 | 1.00 21.67 |
| | | | | 674 674 | | 7.458 | | 1.00 19.18 |
| ATOM | 4561 | NH2 | ARG | 674 | 16.149 | 8.519 | 5.866 | |
| ATOM | 4562 | С | ARG | 674 | 15.045 | 11.264 | -1.917 | 1.00 18.81 |
| ATOM | 4563 | 0 | ARG | 674 | 15.865 | 11.978 | -2.489 | 1.00 17.29 |
| MOTA | 4564 | N | GLY | 675 | 14.250 | 10.418 | -2.568 | 1.00 18.30 |
| MOTA | 4565 | CA | GLY | 675 | 14.338 | 10.292 | -4.013 | 1.00 18.96 |
| MOTA | 4566 | С | GLY | 675 | 13.602 | 11.384 | -4.770 | 1.00 19.21 |
| ATOM | 4567 | 0 | GLY | 675 | 13.982 | 11.737 | -5.890 | 1.00 17.51 |
| ATOM | 4568 | N | ALA | 676 | 12.548 | 11.916 | -4.160 | 1.00 19.23 |
| ATOM | 4569 | CA | ALA | 676 | 11.737 | 12.969 | -4.771 | 1.00 21.38 |
| ATOM | 4570 | СВ | ALA | 676 | . 10.515 | 12.347 | -5.445 | 1.00 22.27 |
| MOTA | 4571 | C | ALA | 676 | 11.291 | 14.003 | -3.731 | 1.00 21.87 |
| | | - | · · | | | • | | |

| ATOM | 4572 | 0 | ALA | 676 | 10.160 | 13.970 | -3.260 | 1.00 21.80 |
|--|--|--------------------------|--|--------------------------|--|-----------------------------------|---|--|
| | | | | | | | | |
| MOTA | 4573 | N | PRO | 677 | 12.174 | 14.951 | -3.376 | 1.00 23.81 |
| MOTA | 4574 | CD | PRO | 677 | 13.544 | 15.130 | -3.888 | 1.00 24.84 |
| ATOM | 4575 | CA | PRO | 677 | 11.854 | 15.984 | -2.384 | 1.00 24.40 |
| ATOM | 4576 | CB | PRO | 677 | 13.204 | 16.654 | -2.140 | 1.00 24.98 |
| | 4577 | CG | PRO | 677 | 13.859 | 16.554 | -3.459 | 1.00 25.58 |
| MOTA | | | | | | | | |
| ATOM | 4578 | С | PRO | 677 | 10.774 | 16.989 | -2.762 | 1.00 23.70 |
| ATOM | 4579 | 0 | PRO | 677 | 10.197 | 17.640 | -1.891 | 1.00 25.65 |
| ATOM | 4580 | N | ASN | 678 | 10.496 | 17.114 | -4.054 | 1.00 24.73 |
| ATOM | 4581 | CA | ASN | 678 | 9.483 | 18.057 | -4.497 | 1.00 24.76 |
| | | | | | | | | |
| MOTA | 4582 | CB | ASN | 678 | 9.994 | 18.852 | -5.706 | 1.00 27.05 |
| ATOM | 4583 | CG | ASN | 678 | 11.256 | 19.634 | -5.395 | 1.00 30.19 |
| ATOM | 4584 | OD1 | ASN | 678 | 11.303 | 20.400 | -4.430 | 1.00 31.87 |
| ATOM | 4585 | ND2 | ASN | 678 | 12.291 | 19.443 | -6.212 | 1.00 31.96 |
| MOTA | 4586 | C | ASN | 678 | 8.164 | 17.385 | -4.845 | 1.00 22.32 |
| | | | | | | | | |
| MOTA | 4587 | 0 | ASN | 678 | 7.206 | 18.056 | -5.205 | 1.00 21.78 |
| MOTA | 4588 | N | CYS | 679 | 8.093 | 16.064 | -4.731 | 1.00 21.57 |
| ATOM | 4589 | CA | CYS | 679 | 6.845 | 15.393 | -5.080 | 1.00 20.82 |
| MOTA | 4590 | CB | CYS | 679 | 7.088 | 13.904 | -5.328 | 1.00 22.07 |
| ATOM | 4591 | SG | CYS | 679 | 6.942 | 12.839 | -3.863 | 1.00 21.95 |
| | | | | | | | | |
| MOTA | 4592 | С | CYS | 679 | 5.761 | 15.549 | -4.017 | 1.00 20.00 |
| ATOM | 4593 | 0 | CYS | 679 | 6.045 | 15.896 | -2.871 | 1.00 20.40 |
| MOTA | 4594 | N | LEU | 680 | 4.513 | 15.336 | -4.432 | 1.00 19.40 |
| ATOM | 4595 | CA | LEU | 680 | 3.380 | 15.365 | -3.520 | 1.00 18.90 |
| ATOM | 4596 | CB | LEU | 680 | 2.074 | 15.699 | -4.242 | 1.00 17.17 |
| | | | | | | | | |
| MOTA | 4597 | CG | LEU | 680 | 0.812 | 15.597 | -3.385 | 1.00 16.51 |
| MOTA | 4598 | CD1 | LEU | 680 | 0.927 | 16.514 | -2.164 | 1.00 17.54 |
| ATOM | 4599 | CD2 | LEU | 680 | -0.406 | 15.947 | -4.211 | 1.00 16.35 |
| ATOM | 4600 | C - | LEU | 680 | 3.354 | 13.917 | -3.056 | 1.00 18.47 |
| ATOM | 4601 | õ | LEU | 680 | 3.069 | 13.014 | -3.846 | 1.00 17.45 |
| | | | | | | | | |
| ATOM | 4602 | N | LEU | 681 | 3.659 | 13.699 | -1.782 | 1.00 18.84 |
| MOTA | 4603 | CA | LEU | 681 | 3.734 | 12.346 | -1.245 | 1.00 18.21 |
| ATOM | 4604 | CB | LEU | 681 | 5.054 | 12.192 | -0.474 | 1.00 18.92 |
| ATOM | 4605 | CG | LEU | 681 | 5.611 | 10.804 | -0.137 | 1.00 20.05 |
| ATOM | 4606 | CD1 | | 681 | 7.014 | 10.970 | 0.436 | 1.00 18.66 |
| | | | | | | | | |
| MOTA | 4607 | CD2 | | 681 | 4.714 | 10.091 | 0.868 | 1.00 21.30 |
| MOTA | 4608 | С | LEU | 681 | 2.566 | 11.966 | -0.353 | 1.00 16.59 |
| ATOM | 4609 | 0 | LEU | 681 | 2.356 | 12.562 | 0.701 | 1.00 16.26 |
| ATOM | 4610 | N | LEU | 682 | 1.802 | 10.974 | -0.790 | 1.00 16.90 |
| | | | | 682 | 0.677 | 10.491 | -0.007 | 1.00 17.13 |
| ATOM | 4611 | CA | LEU | | | | | |
| ATOM | 4612 | СВ | LEU | 682 | -0.520 | 10.151 | -0.900 | 1.00 18.79 |
| ATOM | 4613 | CG | LEU | 682 | -1.449 | 11.291 | -1.333 | 1.00 22.69 |
| ATOM | 4614 | CD1 | LEU | 682 | -0.700 | 12.278 | -2.227 | 1.00 23.30 |
| ATOM | 4615 | CD2 | LEU | 682 | -2.640 | 10.700 | -2.070 | 1.00 23.40 |
| ATOM | 4616 | C | LEU | 682 | 1.156 | 9.233 | 0.690 | 1.00 16.92 |
| | | | | | | | | |
| MOTA | 4617 | 0 | LEU | 682 | 1.870 | 8.430 | 0.098 | 1.00 18.52 |
| MOTA | 4618 | N | ÀΓΑ | 683 | 0.803 | 9.074 | . 1,. 957 | 1.00 14.89 |
| MOTA | 4619 | CA | ALA | 683 | 1.195 | 7.869 | 2.682 | 1.00 14.34 |
| MOTA | 4620 | CB | ALA | 683 | 2.223 | 8.201 | 3.753 | 1.00 14.56 |
| ATOM | 4621 | C | ALA | 683 | -0.049 | 7.260 | 3.308 | 1.00 13.19 |
| | | | | | | | | |
| ATOM | 4622 | 0 | ALA | 683 | -0.893 | 7.967 | 3.857 | 1.00 12.69 |
| ATOM | 4623 | N | ASP | 684 | -0.161 | 5.943 | 3.204 | 1.00 13.76 |
| ATOM | 4624 | CA | ASP | 684 | -1.292 | 5.224 | 3.761 | 1.00 13.79 |
| ATOM | 4625 | CB | ASP | 684 | -1.369 | 3.811 | 3.199 | 1.00 17.15 |
| MOTA | 4626 | CG | ASP | 684 | -2.237 | 3.701 | 1.972 | 1.00 18.93 |
| ATOM | 4627 | | ASP | 684 | -2.988 | 4.647 | 1.660 | 1.00 17.43 |
| | | | | | | | | |
| ATOM | 4628 | | ASP | 684 | -2.174 | 2.630 | 1.334 | 1.00 19.86 |
| ATOM | 4629 | С | ASP | 684 | -1.192 | 5.050 | 5.256 | 1.00 14.01 |
| ATOM | 4630 | 0 | ASP | 684 | -0.098 | 4.854 | 5.791 | 1.00 13.68 |
| MOTA | 4631 | N | LEU | 685 | -2.329 | 5.126 | 5.938 | 1.00 14.34 |
| АТОМ | 4632 | CA | LEU | 685 | -2.335 | 4.819 | 7.359 | 1.00 15.73 |
| | | | | | | | | |
| ATOM | 4633 | CB | LEU | 685 | -3.430 | 5.568 | 8.128 | 1.00 17.73 |
| MOTA | 4634 | CG | LEU | 685 | -3.114 | 7.008 | 8.538 | 1.00 18.92 |
| ATOM | 4635 | CD1 | LEU | 685 | -4.058 | 7.437 | 9.658 | 1.00 20.70 |
| MOTA | 4636 | CD2 | LEU | 685 | -1.670 | 7.106 | 9.013 | 1.00 20.52 |
| MOTA | 4637 | С | LEU | 685 | -2.713 | 3.346 | 7.219 | 1.00 15.76 |
| MOTA | 4638 | ο. | LEU | 685 | -3.731 | 3.022 | 6.616 | 1.00 14.86 |
| | | - | | | | | | |
| ATOM | 4639 | N | PRO | 686 | -1.876 | 2.433 | 7.734 | 1.00 15.32 |
| | | | PRO | 686 | -0.579 | 2.697 | 8.380 | 1.00 16.43 |
| MOTA | 4640 | CD | | 686 | -2.139 | 0.996 | 7.643 | 4 00 46 40 |
| | | CA | PRO | 000 | | | | 1.00 16.10 |
| MOTA | 4640 | | | 686 | -0.80 9 | 0.380 | 8.085 | 1.00 16.10 |
| ATOM ATOM ATOM | 4640 4641 4642 | CA CB | PRO PRO | 686 | | | 8.085 | 1.00 17.06 |
| MOTA MOTA MOTA MOTA | 4640 4641 4642 4643 | CA CB CG | PRO PRO PRO | 686 686 | -0.283 | 1.383 | 8.085 9.073 | 1.00 17.06 1.00 16.35 |
| MOTA MOTA MOTA MOTA | 4640 4641 4642 4643 4644 | CA CB CG C | PRO PRO PRO PRO | 686 686 686 | -0.283 -3.327 | 1.383 | 8.085 9.073 8.458 | 1.00 17.06 1.00 16.35 1.00 16.41 |
| ATOM ATOM ATOM ATOM ATOM ATOM | 4640 4641 4642 4643 4644 4645 | CA CB CG C | PRO PRO PRO PRO PRO | 686 686 686 686 | -0.283 -3.327 -4.008 | 1.383 0.488 1.254 | 8.085 9.073 8.458 9.143 | 1.00 17.06 1.00 16.35 1.00 16.41 1.00 16.37 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 4640 4641 4642 4643 4644 4645 4646 | CA CB CG C N | PRO PRO PRO PRO PRO PHE | 686 686 686 687 | -0.283 -3.327 -4.008 -3.563 | 1.383 0.488 1.254 -0.815 | 8.085 9.073 8.458 9.143 8.358 | 1.00 17.06 1.00 16.35 1.00 16.41 1.00 16.37 1.00 15.03 |
| ATOM ATOM ATOM ATOM ATOM ATOM | 4640 4641 4642 4643 4644 4645 | CA CB CG C | PRO PRO PRO PRO PRO | 686 686 686 686 | -0.283 -3.327 -4.008 -3.563 -4.647 | 1.383 0.488 1.254 | 8.085 9.073 8.458 9.143 | 1.00 17.06 1.00 16.35 1.00 16.41 1.00 16.37 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 4640 4641 4642 4643 4644 4645 4646 | CA CB CG C N | PRO PRO PRO PRO PRO PHE | 686 686 686 687 | -0.283 -3.327 -4.008 -3.563 | 1.383 0.488 1.254 -0.815 | 8.085 9.073 8.458 9.143 8.358 | 1.00 17.06 1.00 16.35 1.00 16.41 1.00 16.37 1.00 15.03 |

| ATOM | 4649 | CG | PHE | 687 | -5.265 | -3.841 | 9.861 | 1.00 15.81 |
|------|------|-----|-----|------------|---------|--------|--------|------------|
| ATOM | 4650 | | PHE | 687 | -6.655 | -3.762 | 9.905 | 1.00 16.16 |
| ATOM | 4651 | | PHE | 687 | -4.619 | -4.758 | 10.685 | 1.00 14.41 |
| ATOM | 4652 | | PHE | 687 | -7.390 | -4.595 | 10.751 | 1.00 16.59 |
| ATOM | 4653 | CE2 | | 687 | -5.337 | -5.597 | 11.535 | 1.00 14.28 |
| ATOM | 4654 | CZ | PHE | 687 | -6.726 | -5.516 | 11.568 | 1.00 18.27 |
| ATOM | 4655 | C | PHE | 687 | -4.663 | -1.106 | 10.538 | 1.00 13.34 |
| | 4656 | o | PHE | 687 | -3.634 | -1.136 | 11.209 | 1.00 13.34 |
| MOTA | | | | | | | | |
| ATOM | 4657 | N | MET | 688 | -5.841 | -0.732 | 11.027 | |
| ATOM | 4658 | CA | MET | 688 | -6.035 | -0.332 | 12.418 | 1.00 14.46 |
| MOTA | 4659 | CB | MET | 688 | -5.922 | -1.558 | 13.340 | 1.00 16.06 |
| MOTA | 4660 | CG | MET | 688 | -6.712 | -1.415 | 14.648 | 1.00 16.59 |
| ATOM | 4661 | SD | MET | 688 | -8.529 | -1.347 | 14.400 | 1.00 16.99 |
| ATOM | 4662 | CE | MET | 688 | -8.858 | -3.054 | 14.056 | 1.00 19.17 |
| MOTA | 4663 | С | MET | 688 | -5.087 | 0.767 | 12.911 | 1.00 14.94 |
| ATOM | 4664 | 0 | MET | 688 | -4.718 | 0.793 | 14.087 | 1.00 18.65 |
| MOTA | 4665 | N | ALA | 689 | -4.680 | 1.676 | 12.031 | 1.00 14.13 |
| ATOM | 4666 | CA | ALA | 689 | -3.803 | 2.765 | 12.466 | 1.00 13.66 |
| MOTA | 4667 | CB | ALA | 689 | -2.719 | 3.034 | 11.421 | 1.00 15.41 |
| MOTA | 4668 | C | ALA | 689 | -4.610 | 4.046 | 12.716 | 1.00 13.55 |
| MOTA | 4669 | 0 | ALA | 689 | -4.051 | 5.085 | 13.051 | 1.00 14.39 |
| MOTA | 4670 | N | TYR | 690 | -5.923 | 3.971 | 12.545 | 1.00 13.83 |
| MOTA | 4671 | CA | TYR | 690 | -6.775 | 5.133 | 12.763 | 1.00 13.76 |
| ATOM | 4672 | CB | TYR | 690 | -7.009 | 5.875 | 11.433 | 1.00 14.18 |
| ATOM | 4673 | CG | TYR | 690 | -7.351 | 4.979 | 10.261 | 1.00 12.90 |
| ATOM | 4674 | CD1 | | 690 | -8.666 | 4.841 | 9.818 | 1.00 12.68 |
| ATOM | 4675 | CE1 | TYR | 690 | -8.981 | 4.004 | 8.741 | 1.00.13.27 |
| ATOM | 4676 | CD2 | TYR | 690 ⋅ | -6.352 | 4.257 | 9.599 | 1.00 13.42 |
| ATOM | 4677 | CE2 | TYR | 690 | -6.651 | 3.418 | 8.526 | 1.00 14.00 |
| ATOM | 4678 | CZ | TYR | 690 | -7.963 | 3.297 | 8.101 | 1.00 13.04 |
| ATOM | 4679 | ОН | TYR | 690 | -8.246 | 2.468 | 7.030 | 1.00 13.04 |
| ATOM | 4680 | C | TYR | 690 | -8.087 | 4.693 | 13.392 | 1.00 14.99 |
| ATOM | 4681 | o | TYR | 690 | -9.166 | 5.144 | 13.005 | 1.00 15.19 |
| ATOM | 4682 | N | ALA | 691 | -7.975 | 3.809 | 14.382 | 1.00 13.19 |
| | 4683 | CA | ALA | 691 | -9.135 | 3.239 | 15.082 | 1.00 13.30 |
| MOTA | | | | | | | - | |
| ATOM | 4684 | CB | ALA | | -8.673 | 2.102 | 15.993 | 1.00 13.88 |
| ATOM | 4685 | C | ALA | 691 | -9.924 | 4.257 | 15.888 | 1.00 13.52 |
| MOTA | 4686 | 0 | ALA | 691 | -11.120 | 4.084 | 16.110 | 1.00 14.21 |
| MOTA | 4687 | N | THR | 692 | -9.235 | 5.293 | 16.354 | 1.00 15.07 |
| ATOM | 4688 | CA | THR | 692 | -9.856 | 6.374 | 17.109 | 1.00 16.94 |
| MOTA | | CB | THR | 692 | -9.608 | 6.268 | 18.629 | 1.00 14.55 |
| ATOM | 4690 | OG1 | THR | 692 | -8.219 | 6.492 | 18.902 | 1.00 15.54 |
| ATOM | 4691 | CG2 | THR | 692 | -10.015 | 4.897 | 19.152 | 1.00 15.71 |
| MOTA | 4692 | C | THR | 692 | -9.165 | 7.635 | 16.636 | 1.00 18.24 |
| MOTA | 4693 | 0 | THR | 692 | -8.080 | 7.576 | 16.059 | 1.00 18.19 |
| ATOM | 4694 | N | PRO | 693 | -9.790 | 8.794 | 16.864 | 1.00 17.17 |
| MOTA | 4695 | CD | PRO | 693 | -11.169 | 8.968 | 17.351 | 1.00 18.47 |
| MOTA | 4696 | CA | PRO | 693 | -9.209 | 10.074 | 16.457 | 1.00 18.57 |
| ATOM | 4697 | CB | PRO | 693 | -10.195 | 11.090 | 17.032 | 1.00 20.23 |
| MOTA | 4698 | CG | PRO | 693 | -11.512 | 10.368 | 16.873 | 1.00 19.28 |
| ATOM | 4699 | C | PRO | 693 | -7.801 | 10.241 | 17.021 | 1.00 18.65 |
| MOTA | 4700 | 0 | PRO | 693 | -6.853 | 10.516 | 16.283 | 1.00 15.76 |
| MOTA | 4701 | N | GLU | 694 | -7.668 | 10.064 | 18.334 | 1.00 18.32 |
| MOTA | 4702 | CA | GLU | 694 | -6.371 | 10.194 | 18.987 | 1.00 21.05 |
| MOTA | 4703 | CB | GLU | 694 | -6.485 | 9.871 | 20.486 | 1.00 24.65 |
| MOTA | 4704 | CG | GLU | 694 | -6.958 | 11.039 | 21.341 | 1.00 32.62 |
| ATOM | 4705 | CD | ĠĿŪ | 694 | -6.747 | 10.804 | 22.832 | 1.00 35.61 |
| ATOM | 4706 | | GLU | 694 | -5.624 | 10.413 | 23.221 | 1.00 40.42 |
| MOTA | 4707 | | GLU | 694 | -7.694 | 11.024 | 23.616 | 1.00 40.47 |
| MOTA | 4708 | С | GLU | 694 | -5.290 | 9.321 | 18.352 | 1.00 18.88 |
| MOTA | 4709 | Ο . | GLU | 694 | -4.156 | 9.766 | 18.181 | 1.00 19.69 |
| MOTA | 4710 | N | GLN | 695 | -5.621 | 8.078 | 18.013 | 1.00 18.90 |
| ATOM | 4711 | CA | GLN | 695 | -4.623 | 7.207 | 17.383 | 1.00 17.55 |
| ATOM | 4712 | CB | GLN | 695 | -5.095 | 5.759 | 17.375 | 1.00 19.52 |
| ATOM | 4713 | CG | GLN | 695 | -5.109 | 5.143 | 18.762 | 1.00 25.76 |
| ATOM | 4714 | CD | GLN | 695 | -5.606 | 3.722 | | 1.00 26.70 |
| ATOM | 4715 | | GLN | 695 | -5.007 | 2.849 | 18.128 | 1.00 28.17 |
| ATOM | 4716 | NE2 | | 695 | -6.709 | 3.477 | 19.455 | 1.00 28.69 |
| ATOM | 4717 | C | GLN | 695 | -4.332 | 7.671 | 15.961 | 1.00 14.39 |
| ATOM | 4718 | 0 | GLN | 695 | -3.197 | 7.598 | 15.498 | 1.00 14.33 |
| ATOM | 4719 | N | ALA | 696 | -5.365 | 8.134 | 15.269 | 1.00 14.25 |
| | | | | 696 | -5.187 | 8.637 | 13.203 | 1.00 13.23 |
| ATOM | 4720 | CA | ALA | | -6.517 | 9.128 | 13.352 | 1.00 12.91 |
| ATOM | 4721 | CB | ALA | 696 | | 9.128 | 13.352 | 1.00 12.84 |
| ATOM | 4722 | C | ALA | 696 696 | -4.184 | | 13.965 | |
| ATOM | 4723 | 0 | ALA | 696 | -3.254 | 9.849 | | 1.00 14.82 |
| MOTA | 4724 | N | PHE | 697 | -4.371 | 10.691 | 14.924 | 1.00 13.95 |
| MOTA | 4725 | CA | PHE | 697 | -3.478 | 11.849 | 15.071 | 1.00 14.74 |
| | | | | | | | | |

| MOTA | 4726 | CB | PHE | 697 | -3.847 | 12.688 | 16.307 | 1.00 14.39 |
|------|------|---------------|-----|-------|--------|---------|--------|------------|
| | | | | | | | | |
| MOTA | 4727 | CG | PHE | 697 | -5.272 | 13.165 | 16.326 | 1.00 14.70 |
| MOTA | 4728 | CD1 | PHE | 697 | -5.973 | 13.364 | 15.138 | 1.00 15.78 |
| ATOM | 4729 | CD2 | PHE | 697 | -5.913 | 13.417 | 17.535 | 1.00 17.31 |
| MOTA | 4730 | CE1 | PHE | 697 | -7.296 | 13.803 | 15.157 | 1.00 17.92 |
| | | CE2 | | 697 | | 13.858 | 17.567 | 1.00 18.65 |
| ATOM | 4731 | | | | -7.235 | | | |
| MOTA | 4732 | \mathbf{cz} | PHE | 697 | -7.928 | 14.050 | 16.373 | 1.00 17.31 |
| MOTA | 4733 | С | PHE | 697 | -2.015 | 11.456 | 15.206 | 1.00 16.50 |
| ATOM | 4734 | 0 | PHE | 697 | -1.155 | 11.972 | 14.491 | 1.00 13.69 |
| | 4735 | | GLU | 698 | | 10.543 | 16.138 | 1.00 15.66 |
| MOTA | | N | | | -1.747 | | | |
| MOTA | 4736 | CA | GLU | 698 | -0.391 | 10.082 | 16.418 | 1.00 17.86 |
| ATOM | 4737 | CB | GLU | 698 | -0.409 | 9.111 | 17.603 | 1.00 21.29 |
| ATOM | 4738 | CG | GLU | 698 | 0.971 | 8.622 | 18.050 | 1.00 30.05 |
| ATOM | 4739 | CD | GLU | 698 | 1.631 | 9.547 | 19.063 | 1.00 34.72 |
| | | | | | | | | |
| MOTA | 4740 | | GLU | 698 | 1.784 | 10.753 | 18.766 | 1.00 37.42 |
| ATOM | 4741 | OE2 | GLU | 698 | 1.998 | 9.064 | 20.165 | 1.00 40.64 |
| MOTA | 4742 | С | GLU | 698 | 0.248 | 9.399 | 15.213 | 1.00 16.35 |
| ATOM | 4743 | 0 | GLU | 698 | 1.385 | 9.702 | 14.836 | 1.00 16.77 |
| | | | | 699 | | 8.473 | 14.614 | 1.00 15.59 |
| MOTA | 4744 | N | ASN | | -0.486 | | | |
| MOTA | 4745 | CA | ASN | 699 | 0.033 | 7.743 | 13.471 | 1.00 15.22 |
| MOTA | 4746 | CB | ASN | 699 | -0.838 | 6.506 | 13.200 | 1.00 14.54 |
| ATOM | 4747 | CG | ASN | 699 | -0.748 | 5.488 | 14.328 | 1.00 17.82 |
| ATOM | 4748 | | ASN | 699 | 0.320 | 5.316 | 14.927 | 1.00 15.96 |
| | | | | | | | | |
| MOTA | 4749 | | ASN | 699 | -1.857 | 4.809 | 14.621 | 1.00 15.38 |
| ATOM | 4750 | C | ASN | 699 | 0.159 | 8.636 | 12.236 | 1.00 14.83 |
| ATOM | 4751 | 0 | ASN | 699 | 1.134 | 8.535 | 11.488 | 1.00 14.23 |
| ATOM | 4752 | N | ALA | 700 | -0.802 | 9.529 | 12.026 | 1.00 14.50 |
| | | | ALA | 700 | -0.710 | 10.431 | 10.880 | 1.00 15.69 |
| MOTA | 4753 | CA | | | | | | |
| MOTA | 4754 | CB | ALA | 700 | -1.961 | 11.288 | 10.781 | 1.00 14.56 |
| ATOM | 4755 | С | ALA | 700 | 0.525 | 11.316 | 11.044 | 1.00 15.36 |
| MOTA | 4756 | 0 | ALA | 700 | 1.253 | 11.555 | 10.089 | 1.00 14.90 |
| ATOM | 4757 | N | ALA | 701 | 0.770 | 11.793 | 12.262 | 1.00 15.92 |
| | | | | | | | | |
| MOTA | 4758 | CA | ALA | 701 | 1.920 | 12.659 | 12.499 | 1.00 16.05 |
| MOTA | 4759 | CB | ALA | 701 | 1.888 | 13.201 | 13.920 | 1.00 15.03 |
| MOTA | 4760 | С | ALA | 701 | 3.232 | .11.930 | 12.244 | 1.00 15.03 |
| ATOM | 4761 | 0 . | ALA | 701 | 4.184 | 12.509 | 11.730 | 1.00 16.35 |
| ATOM | 4762 | N | THR | 702 | 3.289 | 10.657 | 12.612 | 1.00 14.38 |
| | | | | | | | | |
| MOTA | 4763 | | THR | 702 | 4.503 | 9.878 | 12.411 | 1.00 12.85 |
| MOTA | 4764 | CB | THR | 702 | 4.323 | 8.450 | 12.956 | 1.00 12.19 |
| MOTA | 4765 | OG1 | THR | 702 | 4.034 | 8.522 | 14.354 | 1.00 12.71 |
| ATOM | 4766 | CG2 | THR | 702 | 5.577 | 7.625 | 12.744 | 1.00 12.48 |
| | | | | | | | | |
| MOTA | 4767 | C | THR | 702 | 4.861 | 9.817 | 10.928 | 1.00 15.73 |
| ATOM | 4768 | 0 | THR | 702 | 6.015 | 9.991 | 10.549 | 1.00 14.96 |
| MOTA | 4769 | N | VAL | 703 | 3.855 | 9.594 | 10.095 | 1.00 14.32 |
| ATOM | 4770 | CA | VAL | 703 | 4.061 | 9.494 | 8.665 | 1.00 17.24 |
| | | CB | VAL | 703 | 2.825 | 8.862 | 8.019 | 1.00 18.94 |
| MOTA | 4771 | | | | | | | |
| ATOM | 4772 | | VAL | 703 | 2.763 | 9.181 | 6.557 | 1.00 24.70 |
| MOTA | 4773 | CG2 | VAL | 703 | 2.866 | 7.360 | 8.248 | 1.00 17.69 |
| MOTA | 4774 | C | VAL | 703 | 4.373 | 10.850 | 8.037 | 1.00 17.44 |
| ATOM | 4775 | 0 | VAL | 703 | 5.207 | 10.944 | 7.131 | 1.00 17.66 |
| | 4776 | N | MET | 704 | 3.705 | 11.895 | 8.519 | 1.00 15.75 |
| ATOM | | | | | | | | |
| ATOM | 4777 | CA | MET | 704 | 3.942 | 13.246 | 8.020 | 1.00 18.71 |
| MOTA | 4778 | CB. | MET | 704 | 2.926 | 14.231 | 8.615 | 1.00 19.63 |
| ATOM | 4779 | CG | MET | 704 | 1.461 | 13.959 | 8.263 | 1.00 24.43 |
| MOTA | 4780 | SD | MET | 704 | 1.046 | 14.259 | 6.517 | 1.00 27.09 |
| ATOM | 4781 | CE | MET | 704 | 1.225 | 16.072 | 6.424 | 1.00 25.27 |
| | | | | | | 13.691 | | |
| MOTA | 4782 | С | MET | 704 | 5.373 | | 8.379 | |
| ATOM | 4783 | 0 | MET | 704 | 6.075 | 14.240 | 7.534 | 1.00 15.47 |
| ATOM | 4784 | N | ARG | 705 | 5.810 | 13.459 | 9.619 | 1.00 16.57 |
| MOTA | 4785 | CA | ARG | 705 | 7.160 | 13.856 | 10.007 | 1.00 17.21 |
| ATOM | 4786 | CB | ARG | 705 | 7.424 | 13.597 | 11.499 | 1.00 18.12 |
| | | | ARG | | | | 12.470 | 1.00 17.42 |
| MOTA | 4787 | CG | | 705 | 6.566 | 14.413 | | |
| MOTA | 4788 | CD | ARG | 705 | 7.139 | 14.379 | 13.887 | 1.00 18.37 |
| MOTA | 4789 | NE | ARG | 705 | 6.188 | 14.923 | 14.862 | 1.00 21.69 |
| ATOM | 4790 | CZ | ARG | 705 | 5.169 | 14.242 | 15.377 | 1.00 21.26 |
| MOTA | 4791 | | ARG | 705 | 4.960 | 12.980 | 15.024 | 1.00 23.11 |
| | | | | | | | 16.225 | 1.00 22.67 |
| ATOM | 4792 | | ARG | 705 | 4.340 | 14.830 | | |
| ATOM | 4793 | С | ARG | 705 | 8.196 | 13.104 | 9.193 | 1.00 17.07 |
| ATOM | 4794 | 0 | ARG | 705 | 9.330 | 13.568 | 9.027 | 1.00 17.74 |
| ATOM | 4795 | N | ALA | 706 | 7.807 | 11.942 | 8.682 | 1.00 16.11 |
| ATOM | 4796 | CA | ALA | 706 | 8.709 | 11.112 | 7.891 | 1.00 15.58 |
| | | | | | | | | |
| ATOM | 4797 | CB | ALA | 706 | 8.235 | 9.662 | 7.921 | 1.00 14.95 |
| MOTA | 4798 | С | ALA | 706 | 8.847 | 11.584 | 6.445 | 1.00 15.19 |
| ATOM | 4799 | 0 | ALA | 706 | 9.688 | 11.068 | 5.709 | 1.00 15.93 |
| ATOM | 4800 | N | GLY | 707 | 8.022 | 12.544 | 6.033 | 1.00 14.94 |
| ATOM | 4801 | CA | GLY | 707 | 8.130 | 13.053 | 4.677 | 1.00 15.89 |
| | | | | 707 | 6.853 | 13.203 | 3.871 | 1.00 16.03 |
| MOTA | 4802 | С | GLY | , , , | 0.000 | 15.205 | 5.0/1 | 1.00 10.00 |
| | | | | | | | | |

| ATOM | 4803 | 0 | GLY | 707 | 6.851 | 13.882 | 2.843 | 1.00 17.90 |
|------|------|------|-----|------|--------------------|--------|--------|------------|
| ATOM | 4804 | N | ALA | 708 | 5.764 | 12.591 | 4.321 | 1.00 15.28 |
| ATOM | 4805 | CA | ALA | 708 | 4.500 | 12.675 | 3.598 | 1.00 14.65 |
| ATOM | 4806 | СВ | ALA | 708 | 3.524 | 11.646 | 4.140 | 1.00 11.62 |
| ATOM | 4807 | C | ALA | 708 | 3.870 | 14.060 | 3.677 | 1.00 15.64 |
| | 4808 | 0 | ALA | 708 | 4.102 | 14.809 | 4.628 | 1.00 14.42 |
| MOTA | | N | ASN | 709 | 3.061 | 14.394 | 2.675 | 1.00 14.42 |
| MOTA | 4809 | | | | | | 2.660 | 1.00 10.20 |
| MOTA | 4810 | CA | ASN | 709 | 2.369 | 15.682 | | · · |
| MOTA | 4811 | CB | ASN | 709 | 2.482 | 16.363 | 1.297 | 1.00 16.35 |
| ATOM | 4812 | CG | ASN | 709 | 3.905 | 16.548 | 0.855 | 1.00 16.63 |
| MOTA | 4813 | OD1 | | 709 | 4.693 | 17.223 | 1.518 | 1.00 19.11 |
| ATOM | 4814 | ND2 | | 709 | 4.246 | 15.951 | -0.271 | 1.00 13.26 |
| MOTA | 4815 | C | ASN | 709 | 0.890 | 15.455 | 2.931 | 1.00 17.83 |
| MOTA | 4816 | 0 | ASN | 709 | 0.163 | 16.388 | 3.252 | 1.00 18.60 |
| MOTA | 4817 | N. | MET | 710 | 0.448 | 14.212 | 2.779 | 1.00 17.20 |
| MOTA | 4818 | CA | MET | 710 | -0.955 | 13.871 | 2.969 | 1.00 16.87 |
| MOTA | 4819 | CB | MET | 710 | -1.713 | 14.127 | 1.654 | 1.00 18.60 |
| MOTA | 4820 | CG | MET | 710 | -3.200 | 13.816 | 1.659 | 1.00 20.01 |
| MOTA | 4821 | SD | MET | 710 | -3.944 | 14.052 | -0.001 | 1.00 21.60 |
| MOTA | 4822 | CE | MET | 710 | -4.743 | 15.673 | 0.168 | 1.00 23.23 |
| ATOM | 4823 | С | MET | 710 | -1.065 | 12.405 | 3.377 | 1.00 16.40 |
| ATOM | 4824 | 0 | MET | 710 | -0.177 | 11.604 | 3.085 | 1.00 14.55 |
| ATOM | 4825 | N | VAL | 711 | -2.152 | 12.070 | 4.065 | 1.00 16.03 |
| ATOM | 4826 | CA | VAL | 711 | -2.391 | 10.712 | 4.528 | 1.00 16.57 |
| ATOM | 4827 | CB | VAL | 711 | -2.552 | 10.697 | 6.065 | 1.00 19.08 |
| ATOM | 4828 | CG1 | | 711 | -3.021 | 9.352 | 6.515 | 1.00 23.70 |
| ATOM | 4829 | CG2 | VAL | 711 | -1.230 | 11.054 | 6.730 | 1.00 17.88 |
| ATOM | 4830 | C | VAL | 711 | -3.655 | 10.132 | 3.896 | 1.00 17.86 |
| | | | VAL | 711 | -4.635 | 10.152 | 3.690 | 1.00 13.00 |
| ATOM | 4831 | 0 | | | -3.631 | 8.840 | | 1.00 14.07 |
| ATOM | 4832 | N | LYS | 712 | | | 3.570 | |
| ATOM | 4833 | CA | LYS | 712 | -4.798 | 8.187 | 2.985 | 1.00 14.28 |
| ATOM | 4834 | CB | LYS | 712 | -4.445 | 7.501 | 1.648 | 1.00 14.48 |
| ATOM | 4835 | CG · | LYS | 712 | -5.645 | 6.773 | 1.006 | 1.00 13.64 |
| ATOM | 4836 | CD | LYS | 712 | -5.475 | 6.476 | -0.491 | 1.00 14.90 |
| ATOM | 4837 | CE | LYS | 712 | -4.471 | 5.361 | -0.770 | 1.00 14.70 |
| ATOM | 4838 | NZ | ĻYS | 712 | -4.882 | 4.059 | -0.157 | 1.00 15.92 |
| MOTA | 4839 | С | LYS | 712 | -5.371 | 7.160 | 3.960 | 1.00 15.39 |
| MOTA | 4840 | 0 | LYS | 712 | -4.632 | 6.361 | 4.532 | 1.00 13.66 |
| MOTA | 4841 | N | ILE | 713 | -6.683 | 7.203 | 4.167 | 1.00 15.54 |
| ATOM | 4842 | CA | ILE | 713 | -7.349 | 6.260 | 5.060 | 1.00 16.63 |
| MOTA | 4843 | CB | ILE | 713 | -7.800 | 6.949 | 6.379 | 1.00 18.02 |
| ATOM | 4844 | CG2 | ILE | 713 | -6.584 | 7.372 | 7.181 | 1.00 19.14 |
| MOTA | 4845 | CG1 | ILE | 713 | -8.667 | 8.173 | 6.072 | 1.00 20.03 |
| MOTA | 4846 | CD1 | ILE | 713 | -9.130 | 8.925 | 7.332 | 1.00 19.76 |
| ATOM | 4847 | C · | ILE | 713 | -8.553 | 5.642 | 4.351 | 1.00 18.46 |
| ATOM | 4848 | 0 | ILE | 713 | -9.224 | 6.306 | 3.561 | 1.00 17.02 |
| ATOM | 4849 | N | GLU | 714 | -8.809 | 4.363 | 4.622 | 1.00 17.38 |
| ATOM | 4850 | CA | GLU | 714 | -9.917 | 3.642 | 3.995 | 1.00 18.87 |
| ATOM | 4851 | CB | GLU | 714 | -9.530 | 2.180 | 3.735 | 1.00 18.90 |
| ATOM | 4852 | CG | GLU | 714 | -8.183 | 1.990 | 3.074 | 1.00 22.06 |
| ATOM | 4853 | CD | GLU | 714 | -7.866 | 0.530 | 2.797 | 1.00 23.62 |
| ATOM | 4854 | | GLU | 714 | -8.597 | -0.357 | 3.292 | 1.00 22.57 |
| ATOM | 4855 | | GLU | 714 | -6.876 | 0.267 | 2.082 | 1.00 26.90 |
| ATOM | 4856 | C | GLU | .714 | -11.162 | 3.649 | 4.867 | 1.00 18.79 |
| ATOM | 4857 | 0 | GLU | 714 | -11.091 | 3.389 | 6.069 | 1.00 17.88 |
| ATOM | 4858 | N | GLY | 715 | -12.304 | 3.940 | 4.256 | 1.00 17.00 |
| | 4859 | CA | GLY | 715 | -13.545 | 3.956 | 5.002 | 1.00 20.89 |
| MOTA | | | | 715 | -14.476 | 5.056 | 4.553 | 1.00 21.05 |
| MOTA | 4860 | C | GLY | | | | 3.855 | 1.00 21.03 |
| MOTA | 4861 | 0 | GLY | 715 | -14.063 -15.738 | 5.980 | | |
| ATOM | 4862 | N | GLY | 716 | | 4.953 | 4.958 | 1.00 21.69 |
| MOTA | 4863 | CA | GLY | 716 | -16.723 | 5.954 | 4.585 | 1.00 20.54 |
| MOTA | 4864 | C | GLY | 716 | -17.198 | 6.833 | 5.731 | 1.00 19.68 |
| ATOM | 4865 | 0 | GLY | 716 | -16.396 | 7.349 | 6.503 | 1.00 18.63 |
| ATOM | 4866 | N | GLU | 717 | -18.513 | 7.004 | 5.828 | 1.00 20.60 |
| ATOM | 4867 | CA | GLU | 717 | -19.143 | 7.828 | 6.857 | 1.00 23.06 |
| ATOM | 4868 | CB | GLU | 717 | -20.631 | 7.498 | 6.948 | 1.00 26.89 |
| ATOM | 4869 | CG | GLU | 717 | -21.512 | 8.436 | 6.154 | 1.00 35.80 |
| MOTA | 4870 | CD | GLU | 717 | -21.970 | 9.634 | 6.959 | 1.00 37.28 |
| ATOM | 4871 | OE1 | GLU | 717 | -21.125 | 10.277 | 7.616 | 1.00 39.12 |
| MOTA | 4872 | OE2 | GLU | 717 | -23.183 | 9.932 | 6.925 | 1.00 39.31 |
| MOTA | 4873 | C | GLU | 717 | -18.562 | 7.785 | 8.257 | 1.00 21.97 |
| ATOM | 4874 | 0 | GLU | 717 | -18.327 | 8.830 | 8.865 | 1.00 20.61 |
| MOTA | 4875 | N | TRP | 718 | -18.340 | 6.587 | 8.788 | 1.00 20.43 |
| ATOM | 4876 | CA. | TRP | 718 | -17.813 | 6.487 | 10.145 | 1.00 18.97 |
| ATOM | 4877 | СВ | TRP | 718 | -17.553 | 5.019 | 10.527 | 1.00 16.93 |
| ATOM | 4878 | CG | TRP | 718 | -16.338 | 4.387 | 9.900 | 1.00 17.31 |
| ATOM | 4879 | CD2 | TRP | 718 | -15.033 | 4.287 | 10.481 | 1.00 15.20 |

| ATOM | 4880 | CE2 | TRP | 718 | -14.213 | 3.604 | 9.554 | 1.00 17.66 |
|------|------|-----|-----|-----|------------------|--------|---------|------------|
| ATOM | 4881 | CE3 | TRP | 718 | -14.475 | 4.707 | 11.698 | 1.00 16.72 |
| ATOM | 4882 | CD1 | TRP | 718 | -16.260 | 3.780 | 8.677 | 1.00 16.47 |
| ATOM | 4883 | NE1 | | 718 | -14.986 | 3.305 | 8.462 | 1.00 17.35 |
| ATOM | 4884 | CZ2 | TRP | 718 | -12.863 | 3.332 | 9.804 | 1.00 17.75 |
| ATOM | 4885 | CZ3 | TRP | 718 | -13.133 | 4.436 | 11.947 | 1.00 18.17 |
| ATOM | 4886 | CH2 | TRP | 718 | -12.342 | 3.753 | 11.001 | 1.00 18.73 |
| ATOM | 4887 | C | TRP | 718 | -16.554 | 7.318 | 10.372 | 1.00 17.36 |
| ATOM | 4888 | ō | TRP | 718 | -16.263 | 7.697 | 11.504 | 1.00 16.96 |
| ATOM | 4889 | N | LEU | 719 | -15.829 | 7.624 | 9.295 | 1.00 17.61 |
| ATOM | 4890 | CA | LEU | 719 | -14.587 | 8.398 | 9.392 | 1.00 16.01 |
| ATOM | 4891 | CB | LEU | 719 | -13.634 | 7.998 | 8.264 | 1.00 19.58 |
| ATOM | 4892 | CG | LEU | 719 | -12.805 | 6.729 | 8.475 | 1.00 20.53 |
| ATOM | 4893 | | LEU | 719 | -12.035 | 6.426 | 7.205 | 1.00 20.90 |
| ATOM | 4894 | | LEU | 719 | -11.869 | 6.919 | 9.657 | 1.00 21.41 |
| ATOM | 4895 | C | LEU | 719 | -14.722 | 9.918 | 9.385 | 1.00 16.42 |
| ATOM | 4896 | 0 | LEU | 719 | -13.726 | 10.625 | 9.538 | 1.00 15.51 |
| ATOM | 4897 | N | VAL | 720 | -15.938 | 10.425 | 9.225 | 1.00 15.73 |
| ATOM | 4898 | CA | VAL | 720 | -16.154 | 11.869 | 9.181 | 1.00 16.54 |
| ATOM | 4899 | CB | VAL | 720 | -17.664 | 12.201 | 9.174 | 1.00 16.38 |
| ATOM | 4900 | CG1 | VAL | 720 | -17.875 | 13.699 | 9.349 | 1.00 16.79 |
| MOTA | 4901 | | VAL | 720 | -18.283 | 11.734 | 7.867 | 1.00 18.53 |
| ATOM | 4902 | С | VAL | 720 | -15.478 | 12.644 | 10.306 | 1.00 15.87 |
| ATOM | 4903 | 0 | VAL | 720 | -14.713 | 13.572 | 10.045 | 1.00 15.80 |
| ATOM | 4904 | N | GLU | 721 | -15.745 | 12.268 | 11.552 | 1.00 15.71 |
| MOTA | 4905 | CA | GLU | 721 | -15.133 | 12.966 | 12.680 | 1.00 16.66 |
| | 4906 | CB | GLU | 721 | -15.589 | 12.346 | 14.003 | 1.00 18.48 |
| ATOM | 4907 | CG | GLU | 721 | -14.947 | 12.976 | 15.227 | 1.00 22.68 |
| MOTA | 4908 | CD | GLU | 721 | -15.367 | 12.293 | 16.516 | 1.00 25.74 |
| ATOM | 4909 | OE1 | GLU | 721 | -14.966 | 11.131 | 16.732 | 1.00 27.93 |
| ATOM | 4910 | OE2 | GLU | 721 | -16.107 | 12.920 | 17.303 | 1.00 27.98 |
| ATOM | 4911 | С | GLU | 721 | -13.610 | 12.935 | 12.606 | 1.00 15.34 |
| ATOM | 4912 | 0 | GLU | 721 | -12.951 | 13.942 | 12.857 | 1.00 14.72 |
| ATOM | 4913 | N | THR | 722 | -13.055 | 11.772 | 12.274 | 1.00 14.80 |
| ATOM | 4914 | CA | THR | 722 | -11.608 | 11.624 | 12.175 | 1.00 14.47 |
| ATOM | 4915 | СВ | THR | 722 | -11.213 | 10.164 | 11.860 | 1.00 16.94 |
| ATOM | 4916 | OG1 | THR | 722 | -11.580 | 9.322 | 12.964 | 1.00 19.05 |
| ATOM | 4917 | CG2 | THR | 722 | ~9.710 | 10.057 | 11.628 | 1.00 15.42 |
| ATOM | 4918 | C | THR | 722 | -11.034 | 12.536 | 11.099 | 1.00 15.01 |
| MOTA | 4919 | 0 | THR | 722 | -10.001 | 13.167 | 11.299 | 1.00 14.67 |
| MOTA | 4920 | N | VAL | 723 | -11.703 | 12.606 | 9.954 | 1.00 16.05 |
| ATOM | 4921 | CA | VAL | 723 | -11.233 | 13.466 | 8.867 | 1.00 15.71 |
| ATOM | 4922 | CB | VAL | 723 | -12.058 | 13.236 | 7.587 | 1.00 15.17 |
| MOTA | 4923 | CG1 | VAL | 723 | -11.612 | 14.206 | 6.486 | 1.00 14.07 |
| ATOM | 4924 | CG2 | VAL | 723 | -11.880 | 11.807 | 7.122 | 1.00 15.82 |
| ATOM | 4925 | C | VAL | 723 | -11.307 | 14.943 | 9.268 | 1.00 16.42 |
| ATOM | 4926 | 0 | VAL | 723 | -10.353 | 15.694 | , 9.079 | 1.00 16.04 |
| ATOM | 4927 | N | GLN | 724 | -12.437 | 15.354 | 9.831 | 1.00 18.63 |
| MOTA | 4928 | CA | GLN | 724 | -12.599 | 16.743 | 10.241 | 1.00 19.28 |
| MOTA | 4929 | CB | GLN | 724 | -13.980 | 16.955 | 10.869 | 1.00 22.80 |
| MOTA | 4930 | CG | GLN | 724 | -15.145 | 16.539 | 9.983 | 1.00 27.70 |
| MOTA | 4931 | CD | GLN | 724 | -16.488 | 16.695 | 10.675 | 1.00 30.60 |
| MOTA | 4932 | | GLN | 724 | -16.669 | 16.241 | 11.806 | 1.00 32.97 |
| MOTA | 4933 | | GLN | 724 | -17.440 | 17.328 | 9.996 | 1.00 32.67 |
| MOTA | 4934 | С | GLN | 724 | -11.513 | 17.132 | 11.241 | 1.00 19.06 |
| MOTA | 4935 | 0 | GLN | 724 | -10.880 | 18.180 | 11.107 | 1.00 16.76 |
| MOTA | 4936 | N | MET | 725 | -11.288 | 16.283 | 12.239 | 1.00 15.76 |
| MOTA | 4937 | CA | MET | 725 | -10.280 | 16.576 | 13.254 | 1.00 15.65 |
| MOTA | 4938 | CB | MET | 725 | -10.440 | 15.634 | 14.445 | 1.00 14.12 |
| | 4939 | CG | MET | 725 | -11.733 | 15.858 | 15.188 | 1.00 17.99 |
| MOTA | 4940 | SD | MET | 725 | -11.866 | 14.852 | 16.672 | 1.00 21.90 |
| ATOM | 4941 | CE | MET | 725 | -10.847 | 15.827 | 17.760 | 1.00 19.31 |
| MOTA | 4942 | C | MET | 725 | -8.849 | 16.537 | 12.744 | 1.00 14.34 |
| MOTA | 4943 | 0 | MET | 725 | -8.018 | 17.336 | 13.171 | 1.00 14.82 |
| MOTA | 4944 | N | LEU | 726 | -8.553 | 15.615 | 11.834 | 1.00 13.91 |
| MOTA | 4945 | CA | LEU | 726 | -7.207 | 15.540 | 11.292 | 1.00 15.00 |
| MOTA | 4946 | CB | LEU | 726 | -7.067 | 14.333 | 10.366 | 1.00 13.52 |
| ATOM | 4947 | CG | LEU | 726 | -6.658 | 13.016 | 11.034 | 1.00 15.57 |
| ATOM | 4948 | | LEU | 726 | -6.916 | 11.860 | 10.087 | 1.00 15.92 |
| ATOM | 4949 | | LEU | 726 | -5.205 | 13.077 | 11.443 | 1.00 15.18 |
| ATOM | 4950 | C | LEU | 726 | -6.873 | 16.819 | 10.526 | 1.00 16.85 |
| MOTA | 4951 | 0 | LEU | 726 | -5.783 | 17.376 | 10.664 | 1.00 16.74 |
| MOTA | 4952 | N | THR | 727 | -7.822 | 17.275 | 9.716 | 1.00 17.73 |
| ATOM | 4953 | CA | THR | 727 | -7.640 | 18.482 | 8.909 | 1.00 22.25 |
| ATOM | 4954 | CB | THR | 727 | -8.885 -0.135 | 18.755 | 8.050 | 1.00 23.64 |
| ATOM | 4955 | OG1 | | 727 | -9.135 -9.669 | 17.618 | 7.207 | 1.00 25.71 |
| ATOM | 4956 | CG2 | THR | 727 | -8.669 | 19.989 | 7.171 | 1.00 26.68 |

| ATOM | 4957 | С | THR | 727 | -7.332 | 19.719 | 9.747 | 1.00 22.81 |
|--------|------|-----|-----|-----|---------|--------|--------|------------|
| | | Ô | THR | 727 | -6.363 | 20.442 | 9.473 | 1.00 22.47 |
| MOTA | 4958 | | | | | | | |
| ATOM | 4959 | N | GLU | 728 | -8.143 | 19.968 | 10.769 | 1.00 23.34 |
| MOTA | 4960 | CA | GLU | 728 | -7.903 | 21.131 | 11.621 | 1.00 25.65 |
| MOTA | 4961 | CB | GLU | 728 | -9.052 | 21.331 | 12.623 | 1.00 28.30 |
| ATOM | 4962 | CG | GLU | 728 | -9.655 | 20.064 | 13.186 | 1.00 30.71 |
| ATOM | 4963 | CD | GLU | 728 | -10.802 | 20.348 | 14.159 | 1.00 33.29 |
| | | | GLU | 728 | -11.541 | 21.333 | 13.952 | 1.00 35.04 |
| MOTA | 4964 | | | | | | | |
| MOTA | 4965 | OE2 | | 728 | -10.979 | 19.579 | 15.124 | 1.00 32.42 |
| MOTA | 4966 | С | GLU | 728 | -6.570 | 21.013 | 12.353 | 1.00 24.86 |
| MOTA | 4967 | 0 | GLU | 728 | -6.069 | 21.993 | 12.898 | 1.00 25.47 |
| ATOM | 4968 | N | ARG | 729 | -5.986 | 19.816 | 12.353 | 1.00 24.34 |
| ATOM | 4969 | CA | ARG | 729 | -4.700 | 19.612 | 13.010 | 1.00 22.72 |
| | | | | | | | | |
| ATOM | 4970 | СВ | ARG | 729 | -4.757 | 18.372 | 13.907 | 1.00 20.17 |
| MOTA | 4971 | CG | ARG | 729 | -5.646 | 18.597 | 15.121 | 1.00 18.27 |
| MOTA | 4972 | CD | ARG | 729 | -5.986 | 17.326 | 15.876 | 1.00 16.32 |
| MOTA | 4973 | NE | ARG | 729 | -6.862 | 17.615 | 17.011 | 1.00 17.63 |
| ATOM | 4974 | CZ | ARG | 729 | -8.095 | 18.109 | 16.911 | 1.00 19.57 |
| ATOM | 4975 | | ARG | 729 | -8.621 | 18.374 | 15.725 | 1.00 20.07 |
| | | | | | | | | |
| MOTA | 4976 | NH2 | ARG | 729 | -8.808 | 18.350 | 18.003 | 1.00 20.63 |
| MOTA | 4977 | С | ARG | 729 | -3.554 | 19.524 | 12.004 | 1.00 22.25 |
| MOTA | 4978 | 0 | ARG | 729 | -2.546 | 18.855 | 12.232 | 1.00 21.75 |
| MOTA | 4979 | N | ALA | 730 | -3.737 | 20.211 | 10.880 | 1.00 22.50 |
| MOTA | 4980 | CA | ALA | 730 | -2.732 | 20.296 | 9.825 | 1.00 21.57 |
| MOTA | 4981 | СВ | ALA | 730 | -1.419 | 20.801 | 10.417 | 1.00 20.27 |
| | | | | | | | | |
| MOTA | 4982 | С | ALA | 730 | -2.472 | 19.044 | 9.008 | 1.00 19.61 |
| ATOM . | 4983 | 0 | ALA | 730 | -1.474 | 18.978 | 8.301 | 1.00 18.88 |
| MOTA | 4984 | N | VAL | 731 | -3.356 | 18.057 | 9.083 | 1.00 17.78 |
| ATOM | 4985 | CA | VAL | 731 | -3.136 | 16.846 | 8.308 | 1.00 17.66 |
| ATOM | 4986 | СВ | VAL | 731 | -3.204 | 15.596 | 9.205 | 1.00 17.57 |
| | | | | | -2.985 | 14.339 | 8.363 | 1.00 16.76 |
| MOTA | 4987 | | VAL | 731 | | | | |
| MOTA | 4988 | CG2 | VAL | 731 | -2.138 | 15.688 | 10.296 | 1.00 18.90 |
| ATOM | 4989 | С | VAL | 731 | -4.114 | 16.673 | 7.153 | 1.00 17.88 |
| MOTA | 4990 | 0 | VAL | 731 | -5.283 | 16.373 | 7.365 | 1.00 17.43 |
| ATOM | 4991 | N | PRO | 732 | -3.652 | 16.892 | 5.912 | 1.00 17.50 |
| ATOM | 4992 | CD | PRO | 732 | -2.351 | 17.419 | 5.475 | 1.00 19.31 |
| ATOM | 4993 | CA | PRO | 732 | -4.554 | 16.727 | 4.773 | 1.00 18.43 |
| | | | | | | | | |
| ATOM | 4994 | CB | PRO | 732 | -3.771 | 17.325 | 3.607 | |
| MOTA | 4995 | CG | PRO | 732 | -2.359 | 17.103 | 4.002 | 1.00 23.17 |
| ATOM | 4996 | С | PRO | 732 | -4.820 | 15.248 | 4.606 | 1.00 16.61 |
| ATOM | 4997 | 0 | PRO | 732 | -3.927 | 14.415 | 4.797 | 1.00 15.91 |
| ATOM | 4998 | N | VAL | 733 | -6.056 | 14.925 | 4.257 | 1.00 15.66 |
| ATOM | 4999 | CA | VAL | 733 | -6.466 | 13.538 | 4.101 | 1.00 16.50 |
| | | | | | | | | |
| ATOM | 5000 | CB. | VAL | 733 | -7.543 | 13.184 | 5.144 | |
| MOTA | 5001 | | VAL | 733 | -7.868 | 11.690 | 5.069 | 1.00 21.58 |
| MOTA | 5002 | CG2 | VAL | 733 | -7.070 | 13.588 | 6.541 | 1.00 17.55 |
| ATOM | 5003 | С | VAL | 733 | -7.038 | 13.185 | 2.737 | 1.00 16.46 |
| ATOM | 5004 | 0 | VAL | 733 | -7.803 | 13.951 | 2.160 | 1.00 16.24 |
| ATOM | 5005 | N | CYS | 734 | -6.668 | 12.010 | 2.242 | 1.00 13.15 |
| | 5006 | CA | CYS | 734 | -7.184 | 11.490 | 0.983 | 1.00 13.80 |
| ATOM | | | | | | | | |
| MOTA | 5007 | CB | CYS | 734 | -6.051 | 10.957 | 0.120 | 1.00 11.02 |
| ATOM | 5008 | SG | CYS | 734 | -6.600 | 10.069 | -1.355 | 1.00 15.01 |
| ATOM | 5009 | C | CYS | 734 | -8.075 | 10.324 | 1.397 | 1.00 14.24 |
| MOTA | 5010 | 0 | CYS | 734 | -7.641 | 9.453 | 2.150 | 1.00 16.01 |
| ATOM | 5011 | N | GLY | 735 | -9.314 | 10.323 | 0.921 | 1.00 12.03 |
| ATOM | 5012 | CA | GLY | 735 | -10.229 | 9.250 | 1.246 | 1.00 13.47 |
| | | | | | -9.985 | | | 1.00 13.47 |
| ATOM | 5013 | С | GLY | 735 | | 8.069 | 0.322 | |
| ATOM | 5014 | 0 | GLY | 735 | -9.214 | 8.174 | -0.630 | 1.00 15.25 |
| MOTA | 5015 | N | HIS | 736 | -10.647 | 6.946 | 0.593 | 1.00 14.52 |
| MOTA | 5016 | CA | HIS | 736 | -10.484 | 5.736 | -0.216 | 1.00 14.30 |
| ATOM | 5017 | CB | HIS | 736 | -9.269 | 4.956 | 0.311 | 1.00 15.08 |
| MOTA | 5018 | CG | HIS | 736 | -8.839 | 3.797 | -0.542 | 1.00 16.75 |
| ATOM | 5019 | | HIS | 736 | -9.519 | 3.010 | -1.411 | 1.00 17.45 |
| | | | | | -7.559 | | | |
| ATOM | 5020 | | HIS | 736 | | 3.287 | -0.488 | 1.00 16.99 |
| ATOM | 5021 | | HIS | 736 | -7.469 | 2.236 | -1.282 | 1.00 18.58 |
| ATOM | 5022 | NE2 | HIS | 736 | -8.645 | 2.045 | -1.854 | 1.00 16.34 |
| ATOM | 5023 | С | HIS | 736 | -11.768 | 4.919 | -0.089 | 1.00 14.46 |
| MOTA | 5024 | 0 | HIS | 736 | -12.096 | 4.441 | 1.000 | 1.00 14.94 |
| ATOM | 5025 | N | LEU | 737 | -12.497 | 4.777 | -1.198 | 1.00 16.18 |
| | | | | | -13.763 | 4.033 | -1.215 | 1.00 17.93 |
| ATOM | 5026 | CA | LEU | 737 | | | | |
| MOTA | 5027 | CB | LEU | 737 | -14.946 | 4.992 | -1.415 | 1.00 16.80 |
| MOTA | 5028 | CG | LEU | 737 | -15.210 | 6.030 | -0.320 | 1.00 13.20 |
| ATOM | 5029 | CD1 | LEU | 737 | -16.249 | 7.044 | -0.807 | 1.00 13.79 |
| ATOM | 5030 | CD2 | LEU | 737 | -15.695 | 5.326 | 0.939 | 1.00 15.41 |
| ATOM | 5031 | C | LEU | 737 | -13.776 | 2.993 | -2.323 | 1.00 18.17 |
| ATOM | 5032 | 0 | LEU | 737 | -12.963 | 3.040 | -3.245 | 1.00 16.22 |
| | | | | | | | | |
| MOTA | 5033 | N | GLY | 738 | -14.715 | 2.060 | -2.223 | 1.00 19.98 |

| ATOM | 5034 | CA | GLY | 738 | | -14.822 | 1.006 | -3.209 | 1.00 | 22.29 |
|------|------|-----|-------|-------|---|---------|---------|--------|------|-------|
| | | | | | | | | | 1.00 | |
| MOTA | 5035 | С | GLY | 738 | | -14.154 | -0.215 | -2.623 | | 23.99 |
| MOTA | 5036 | 0 | GLY | 738 | | -14.432 | -0.588 | -1.487 | | 23.25 |
| MOTA | 5037 | N | LEU | 739 | | -13.257 | -0.822 | -3.390 | 1.00 | 25.38 |
| | 5038 | CA | LEU | 739 | | -12.537 | -1.999 | -2.941 | 1 00 | 25.53 |
| MOTA | | | | | | | | | | |
| MOTA | 5039 | CB | LEU | 739 | | -11.955 | -2.731 | -4.152 | | 26.77 |
| MOTA | 5040 | CG | LEU | 739 | | -11.686 | -4.230 | -4.032 | 1.00 | 28.57 |
| MOTA | 5041 | CD1 | LEU | 739 | | -10.971 | -4.722 | -5.291 | 1.00 | 29.59 |
| | | | | | | | | | | |
| MOTA | 5042 | CD2 | LEU | 739 | | -10.849 | -4.508 | -2.804 | | 27.92 |
| MOTA | 5043 | C | LEU | 739 | | -11.413 | -1.560 | -1.998 | 1.00 | 26.90 |
| ATOM | 5044 | 0 | LEU | 739 | | -10.331 | -1.173 | -2.443 | 1.00 | 27.05 |
| | 5045 | N | | 740 | | -11.686 | -1.605 | -0.697 | | 25.51 |
| MOTA | | | THR | | | | | | | |
| ATOM | 5046 | CA | THR | 740 | | -10.708 | -1.226 | 0.319 | | 26.30 |
| ATOM | 5047 | CB | THR | 740 | | -11.399 | -0.547 | 1.514 | 1.00 | 25.07 |
| ATOM | 5048 | OG1 | THR | 740 | | -12.585 | -1.272 | 1.852 | 1.00 | 26.66 |
| | | | | | | | | | | |
| ATOM | 5049 | CG2 | THR | 740 | | -11.783 | 0.886 | 1.170 | 1.00 | |
| ATOM | 5050 | С | THR | 740 | | -9.986 | -2.487 | 0.794 | 1.00 | 25.33 |
| MOTA | 5051 | 0 | THR | 740 | | -10.522 | -3.252 | 1.594 | 1.00 | 26.61 |
| | | | | 741 | | -8.748 | -2.704 | 0.312 | | 25.06 |
| MOTA | 5052 | N | PRO | | | | | | | |
| MOTA | 5053 | CD | PRO | 741 | | -8.001 | -1.737 | -0.510 | 1.00 | 26.23 |
| MOTA | 5054 | CA | PRO | 741 | | -7.909 | -3.862 | 0.641 | 1.00 | 22.16 |
| ATOM | 5055 | CB | PRO | 741 | | -6.584 | -3.542 | -0.060 | | 25.15 |
| | | | | | | | | | | |
| MOTA | 5056 | CG | PRO | 741 | | -6.588 | -2.048 | -0.144 | | 28.32 |
| MOTA | 5057 | С | PRO | 741 | | -7.736 | -4.223 | 2.111 | 1.00 | 20.97 |
| ATOM | 5058 | 0 | PRO . | 741 | | -7.560 | -5.397 | 2.441 | 1.00 | 20.75 |
| | | | | | | | | | | |
| ATOM | 5059 | N | GLN | 742 | | -7.783 | -3.241 | 3.003 | | 18.98 |
| ATOM | 5060 | CA | GLN | 742 | | -7.637 | -3.556 | 4.425 | 1.00 | 18.22 |
| ATOM | 5061 | CB | GLN . | 742 | | -7.516 | -2.273 | 5.246 | 1.00 | 18.22 |
| ATOM | | | GLN | 742. | | -6.108 | -1.698 | 5.237. | | 19.20 |
| | 5062 | CG | | | | | | | | |
| ATOM | 5063 | CD | GLN | 742 | | -6.037 | -0.295 | 5.799 | 1.00 | 21.99 |
| ATOM | 5064 | OE1 | GLN | 742 | | -6.773 | 0.056 | 6.722 | 1.00 | 23.77 |
| ATOM | 5065 | NE2 | GLN | 742 | | -5.130 | | 5.258 | 1.00 | 19.08 |
| | | | | | | | | | | |
| MOTA | 5066 | С | GLN | 742 | | -8.813 | -4.398 | 4.916 | 1.00 | 17.75 |
| ATOM | 5067 | 0 | GLN | 742 | | -8.659 | -5.212 | 5.826 | 1.00 | 17.97 |
| ATOM | 5068 | N | SER | 743 | | -9.976 | -4.209 | 4.296 | 1.00 | 18.05 |
| | 5069 | CA | SER | 743 | | -11.171 | -4.950 | 4.673 | | 17.66 |
| ATOM | | | | | | | | | | |
| ATOM | 5070 | CB | SER | 743 | | -12.412 | -4.063 | 4.535 | | 19.22 |
| ATOM | 5071 | OG | SER | 743 | | -12.368 | -2.992 | 5.473 | 1.00 | 19.51 |
| ATOM | 5072 | С | SER | 743 | | -11.347 | -6.222 | 3.849 | 1.00 | 18.63 |
| | | | | | | | | | | |
| ATOM | 5073 | 0 | SER | 743 | | -12.456 | -6.742 | 3.725 | 1.00 | 19.29 |
| ATOM | 5074 | N | VAL | 744 | | -10.252 | -6.733 | 3.291 | 1.00 | 17.52 |
| ATOM | 5075 | CA | VAL | 744 | | -10.320 | -7.949 | 2.483 | 1.00 | 18.17 |
| | | | | 744 | | -8.900 | -8.422 | 2.066 | 1.00 | 20.91 |
| MOTA | 5076 | СВ | VAL | | | | | | | |
| ATOM | 5077 | CG1 | VAL | 744 | | -8.072 | -8.777 | 3.294 | 1.00 | 20.41 |
| ATOM | 5078 | CG2 | VAL | 744 | • | -9.004 | -9.617 | 1.126 | 1.00 | 21.66 |
| ATOM | 5079 | C | VAL | 744 | | -11.061 | -9.087 | 3.206 | 1.00 | 18.57 |
| | | | | | | | | | | |
| ATOM | 5080 | 0 | VAL | 744 | | -11.873 | -9.786 | 2.594 | 1.00 | 17.85 |
| MOTA | 5081 | N | ASN | 745 | | -10.801 | -9.267 | 4.501 | 1.00 | 18.34 |
| MOTA | 5082 | CA | ASN | 745 | | -11.451 | -10.337 | 5.256 | 1.00 | 18.99 |
| | | | | | | | | | | |
| ATOM | 5083 | CB | ASN | 745 | | -10.783 | -10.501 | 6.624 | 1.00 | 18.10 |
| ATOM | 5084 | CG | ASN | 745 | | -9.306 | -10.825 | 6.505 | 1.00 | 18.24 |
| ATOM | 5085 | OD1 | ASN | 745 | | -8.931 | -11.911 | 6.055 | 1.00 | 16.42 |
| | 5086 | | ASN | 745 | | -8.462 | -9.882 | 6.890 | 1.00 | 16.58 |
| ATOM | | | | | | | | | | |
| MOTA | 5087 | С | ASN | 745 | | | -10.100 | 5.426 | 1.00 | 20.36 |
| MOTA | 5088 | 0 | ASN | . 745 | | -13.718 | -11.046 | 5.590 | 1.00 | 19.24 |
| ATOM | 5089 | N | ILE | 746 | | -13.352 | -8.835 | 5.385 | 1.00 | 21.75 |
| | | | | | | | -8.474 | | 1.00 | 24.03 |
| MOTA | 5090 | CA | ILE | 746 | | -14.758 | | 5.512 | | |
| MOTA | 5091 | CB | ILE | 746 | | -14.928 | -6.955 | 5.722 | 1.00 | 25.51 |
| ATOM | 5092 | CG2 | ILE | 746 | | -16.393 | -6.570 | 5.577 | 1.00 | 27.38 |
| ATOM | 5093 | CG1 | | 746 | | -14.406 | -6.553 | 7.103 | 1.00 | 25.99 |
| | | | | | | | | | | |
| MOTA | 5094 | CDI | ILE | 746 | | -15.274 | -7.038 | 8.241 | 1.00 | 23.57 |
| ATOM | 5095 | С | ILE | 746 | | -15.481 | -8.866 | 4.233 | 1.00 | 25.01 |
| ATOM | 5096 | 0 | ILE | 746 | | -16.510 | -9.537 | 4.274 | 1.00 | 24.42 |
| | | | | 747 | | -14.927 | -8.450 | 3.098 | 1.00 | 26.24 |
| MOTA | 5097 | N | PHE | | | | | | | |
| ATOM | 5098 | CA | PHE | 747 | | -15.521 | -8.743 | 1.796 | 1.00 | 27.97 |
| ATOM | 5099 | CB | PHE | 747 | | -14.900 | -7.859 | 0.709 | 1.00 | 30.22 |
| ATOM | 5100 | CG | PHE | 747 | | -14.863 | -6.396 | 1.056 | 1.00 | 33.12 |
| | | | | | | | | | | |
| ATOM | 5101 | | PHE | 747 | | -16.006 | -5.739 | 1.504 | 1.00 | 34.45 |
| MOTA | 5102 | CD2 | PHE | 747 | | -13.680 | -5.672 | 0.924 | 1.00 | 34.85 |
| ATOM | 5103 | | PHE | 747 | | -15.970 | -4.380 | 1.819 | 1.00 | 35.58 |
| ATOM | 5104 | CE2 | | 747 | | -13.631 | -4.313 | 1.235 | | 35.40 |
| | | | | | | | | | | |
| MOTA | 5105 | CZ | PHE | 747 | | -14.779 | -3.668 | 1.683 | 1.00 | 35.63 |
| MOTA | 5106 | C | PHE | 747 | | -15.323 | -10.203 | 1.412 | 1.00 | 29.09 |
| ATOM | 5107 | ō | PHE | 747 | | -16.061 | -10.742 | 0.587 | 1.00 | |
| | | | | | | | | | | |
| MOTA | 5108 | N | GLY | 748 | | -14.317 | -10.837 | 2.006 | 1.00 | 29.00 |
| MOTA | 5109 | CA | GLY | 748 | | -14.042 | -12.229 | 1.698 | 1.00 | 29.92 |
| MOTA | 5110 | С | GLY | 748 | | -13.185 | -12.347 | 0.453 | 1.00 | 30.99 |
| | | - | | | | / | | | | |

| ATOM | 5111 | 0 | GLY | 748 | -13 23 | 28 -13.354 | -0.253 | 1.00 33.17 |
|------|------|----------|-----|------|--------|------------|---------|------------|
| | 5112 | N | GLY | 749 | -12.40 | | | 1.00 30.50 |
| MOTA | | | | | | | | |
| MOTA | 5113 | CA | GLY | 749 | -11.53 | | | 1.00 31.40 |
| MOTA | 5114 | С | GLY | 749 | -11.59 | | | 1.00 33.02 |
| MOTA | 5115 | 0 | GLY | 749 | -12.2 | 79 -9.052 | -1.269 | 1.00 31.79 |
| ATOM | 5116 | N | TYR | 750 | -10.85 | 57 -9.862 | -2.807 | 1.00 33.78 |
| ATOM | 5117 | CA | TYR | 750 | -10.83 | | | 1.00 35.38 |
| | | | | | | | | 1.00 36.26 |
| MOTA | 5118 | CB | TYR | 750 | -9.44 | | | |
| ATOM | 5119 | CG | TYR | 750 | -8.36 | | | 1.00 38.04 |
| MOTA | 5120 | CD1 | TYR | 750 | -7.86 | 51 -9.674 | -2.639 | 1.00 39.14 |
| ATOM | 5121 | CE1 | TYR | 750 | -6.88 | 36 -9.742 | -1.644 | 1.00 39.39 |
| ATOM | 5122 | CD2 | TYR | 750 | -7.85 | 58 -7.283 | -2.490 | 1.00 38.52 |
| ATOM | 5123 | CE2 | TYR | 750 | -6.88 | | | 1.00 39.18 |
| | | | | 750 | -6.40 | | | 1.00 39.42 |
| MOTA | 5124 | CZ | TYR | | | | | |
| ATOM | 5125 | ОН | TYR | 750 | -5.44 | | | 1.00 39.23 |
| MOTA | 5126 | С | TYR | 750 | -11.85 | | | 1.00 35.70 |
| MOTA | 5127 | 0 | TYR | 750 | -11.59 | 91 -9.304 | -5.753 | 1.00 36.41 |
| ATOM | 5128 | N | LYS | 751 | -13.02 | 25 -8.127 | -4.480 | 1.00 35.48 |
| ATOM | 5129 | CA | LYS | 751 | -14.09 | | | 1.00 36.67 |
| ATOM | 5130 | CB | LYS | 751 | -15.25 | | | 1.00 38.25 |
| | | | | | | | | |
| MOTA | 5131 | CG | LYS | 751 | -14.83 | | | 1.00 40.62 |
| ATOM | 5132 | CD | LYS | 751 | -15.8 | | | 1.00 42.04 |
| MOTA | 5133 | CE | LYS | 751 | -15.34 | 14 -12.243 | -2.802 | 1.00 42.02 |
| ATOM | 5134 | NZ | LYS | 751 | -16.33 | 34 -12.839 | -1.854 | 1.00 42.38 |
| MOTA | 5135 | C | LYS | 751 | -14.56 | 59 -6.741 | -5.783 | 1.00 36.24 |
| ATOM | 5136 | 0 | LYS | 751 | -14.3 | | | 1.00 36.25 |
| | 5137 | | | 752 | -15.19 | | | 1.00 36.26 |
| MOTA | | N | VAL | | | | | |
| ATOM | 5138 | CA | VAL | 752 | -15.68 | | | 1.00 36.20 |
| MOTA | 5139 | CB | VAL | 752 | -16.19 | | | 1.00 36.16 |
| MOTA | 5140 | CG1 | VAL | 752 | -16.79 | 94 -3.948 | -9.191 | 1.00 36.40 |
| ATOM | 5141 | CG2 | VAL | 752 | -15.05 | 57 -5.641 | -9.753 | 1.00 35.98 |
| ATOM | 5142 | С | VAL | 752 | -16.82 | | | 1.00 36.45 |
| ATOM | 5143 | ō. | VAL | 752 | -17.79 | | | 1.00 36.56 |
| | | | | | | | | 1.00 36.02 |
| MOTA | 5144 | N | GLN | 753 | -16.74 | | | |
| ATOM | 5145 | CA | GLN | 753 | -17.7 | | | 1.00 36.40 |
| ATOM | 5146 | CB | GLN | 753 | -17.15 | 56 -2.319 | -3.915 | 1.00 37.30 |
| ATOM | 5147 | CG | GLN | 753 | -17.03 | 31 -3.264 | -2.730 | 1.00 42.36 |
| ATOM | 5148 | CD | GLN | 753 | -15.99 | 96 -4.345 | -2.946 | 1.00 44.63 |
| ATOM | 5149 | OE1 | | 753 | -14.83 | | | 1.00 46.92 |
| ATOM | 5150 | NE2 | GLN | 753 | -16.42 | | | 1.00 44.11 |
| | | | | | | | | |
| ATOM | 5151 | C | GLN | 753 | -18.54 | | | 1.00 35.82 |
| ATOM | 5152 | 0 | GLN | 753 | -18.13 | | | 1.00 34.76 |
| MOTA | 5153 | N | GLY | 754 | -19.64 | 45 -1.417 | | 1.00 36.54 |
| MOTA | 5154 | CA - | GLY | 754 | -20.44 | 46 -0.397 | -6.015 | 1.00 37.86 |
| MOTA | 5155 | С | GLY | 754 | -21.5 | 71 -0.979 | -6.848 | 1.00 38.80 |
| ATOM | 5156 | 0 | GLY | 754 | -22.5 | 58 -0.301 | | 1.00 38.37 |
| ATOM | 5157 | N | ARG | 755 | -21.43 | | | 1.00 40.53 |
| | | | | 755 | | | | 1.00 42.45 |
| ATOM | 5158 | CA | ARG | | -22.40 | | | |
| MOTA | 5159 | CB | ARG | 755 | -22.01 | | | 1.00 43.43 |
| MOTA | 5160 | CG | ARG | 755 | -20.75 | | | 1.00 44.60 |
| MOTA | 5161 | CD | ARG | 755 | -21.06 | 59 -4.927 | -10.423 | 1.00 44.87 |
| ATOM | 5162 | NE · | ARG | 755 | -19.88 | 33 -5.181 | -11.242 | 1.00 44.38 |
| MOTA | 5163 | CZ | ARG | 755 | -19.04 | 11 -6.196 | -11.066 | 1.00 45.22 |
| ATOM | 5164 | | ARG | 755 | -19.24 | | -10.090 | 1.00 45.18 |
| ATOM | 5165 | NH2 | ARG | 755 | -18.00 | | | 1.00 44.29 |
| | | ~ | | | | | | 1.00 42.83 |
| MOTA | 5166 | C | ARG | 755 | -23.78 | | | |
| MOTA | 5167 | 0 | ARG | 755 | -23.99 | | | 1.00 43.19 |
| MOTA | 5168 | N | GLY | 756 | -24.73 | 34 -2.257 | | 1.00 43.66 |
| ATOM | 5169 | CA | GLY | 756 | -26.0 | 79 -2.103 | -7.616 | 1.00 44.45 |
| MOTA | 5170 | С | GLY | 756 | -26.40 | 04 -0.696 | -7.154 | 1.00 45.42 |
| MOTA | 5171 | 0 | GLY | 756 | -25.53 | | -6.827 | 1.00 45.05 |
| ATOM | 5172 | N | ASP | 757 | -27.69 | | | 1.00 45.36 |
| | | | | | | | | 1.00 45.65 |
| ATOM | 5173 | CA | ASP | 757 | -28.15 | | | |
| MOTA | 5174 | CB | ASP | 757 | -29.64 | | -7.011 | 1.00 48.39 |
| MOTA | 5175 | CG | ASP | 757 | -29.95 | | | 1.00 50.42 |
| MOTA | 5176 | OD1 | ASP | 757 | -29.42 | | | 1.00 51.37 |
| MOTA | 5177 | OD2 | ASP | 757 | -30.72 | 25 -0.051 | -8.795 | 1.00 51.94 |
| MOTA | 5178 | С | ASP | 757 | -27.89 | 98 1.188 | -5.219 | 1.00 43.87 |
| ATOM | 5179 | ō | ASP | 757 | -27.44 | | | 1.00 43.00 |
| ATOM | 5180 | N | GLU | 758 | -28.19 | | | 1.00 42.25 |
| | | | | | -27.98 | | | 1.00 41.44 |
| MOTA | 5181 | CA | GLU | 758 | | | | |
| ATOM | 5182 | CB | GLU | 758 | -28.33 | | | 1.00 43.32 |
| MOTA | 5183 | CG | GLU | 758 | -28.24 | | | 1.00 47.39 |
| MOTA | 5184 | CD | GLU | 758 | -27.79 | | | 1.00 49.85 |
| MOTA | 5185 | OE1 | GLU | 758 | -28.44 | 46 -3.298 | -0.389 | 1.00 50.43 |
| MOTA | 5186 | OE2 | GLU | 758 | -26.79 | 96 -2.248 | 0.632 | 1.00 50.64 |
| ATOM | 5187 | C | GLU | 758 | -26.53 | | | 1.00 39.44 |
| | 520, | _ | | . 30 | | | | |

| MOTA | 5188 | 0 | GLU | 758 | -26.242 | 1.628 | -1.956 | 1.00 37.55 |
|--------------|------|--------|-----|------------|--------------------|------------------|----------------|--------------------------|
| ATOM | 5189 | N | ALA | 759 | -25.622 | -0.160 | -3.180 | 1.00 37.40 |
| ATOM | 5190 | CA | ALA | 759 | -24.191 | 0.037 | -2.981 | 1.00 34.93 |
| ATOM | 5191 | СВ | ALA | 759 | -23.420 | -1.141 | -3.568 | 1.00 35.45 |
| | 5192 | С | ALA | 759 | -23.735 | 1.332 | -3.639 | 1.00 33.43 |
| ATOM | | | | | | | | 1.00 33.03 |
| MOTA | 5193 | 0 | ALA | 759 | -22.993 | 2.114 | -3.045 | |
| MOTA | 5194 | N | GLY | 760 | -24.182 | 1.541 | -4.873 | 1.00 31.34 |
| MOTA | 5195 | CA | GLY | 760 | -23.819 | 2.735 | -5.610 | 1.00 29.95 |
| MOTA | 5196 | C | GLY | 760 | -24.143 | 4.016 | -4.868 | 1.00 29.45 |
| MOTA | 5197 | 0 | GLY | 760 | -23.272 | 4.866 | -4.684 | 1.00 28.24 |
| ATOM | 5198 | N | ASP | 761 | -25.396 | 4.152 | -4.440 | 1.00 28.80 |
| MOTA | 5199 | CA | ASP | 761 | -25.840 | 5.335 | -3.714 | 1.00 28.80 |
| ATOM | 5200 | CB | ASP | 761 | -27.343 | 5.248 | -3.415 | 1.00 29.11 |
| MOTA | 5201 | CG | ASP | 761 | -28.193 | 5.146 | -4.676 | 1.00 29.37 |
| ATOM | 5202 | | ASP | 761 | -27.664 | 5.376 | -5.782 | 1.00 29.25 |
| MOTA' | 5203 | | ASP | 761 | -29.400 | 4.845 | -4.556 | 1.00 31.42 |
| | 5204 | C C | ASP | 761 | -25.070 | 5.494 | -2.410 | 1.00 28.23 |
| ATOM | | | | | | | | 1.00 26.71 |
| MOTA | 5205 | 0 | ASP | 761 | -24.802 | 6.612 | -1.960 | |
| ATOM | 5206 | N | GLN | 762 | -24.717 | 4.369 | -1.798 | 1.00 28.59 |
| MOTA | 5207 | CA | GLN | 762 | -23.970 | 4.396 | -0.546 | 1.00 28.32 |
| MOTA | 5208 | CB | GLN | 762 | -23.858 | 2.988 | 0.040 | 1.00 30.23 |
| MOTA | 5209 | CG | GLN | 762 | -23.020 | 2.931 | 1.305 | 1.00 32.27 |
| MOTA | 5210 | CD | GLN | 762 | -23.535 | 3.860 | 2.378 | 1.00 33.99 |
| MOTA | 5211 | OE1 | GLN | 762 | -24.663 | 3.718 | 2.852 | 1.00 36.79 |
| MOTA | 5212 | NE2 | GLN | 762 | -22.712 | 4.825 | 2.767 | 1.00 35.03 |
| MOTA | 5213 | С | GLN | 762 | -22.571 | 4.973 | -0.754 | 1.00 26.19 |
| ATOM | 5214 | ō | GLN | 762 | -22.091 | 5.757 | 0.065 | 1.00 24.24 |
| ATOM | 5215 | N | LEU | 763 | -21.917 | 4.578 | -1.842 | 1.00 25.52 |
| ATOM | 5216 | CA | LEU | 763 | -20.575 | 5.078 | -2.135 | 1.00 25.74 |
| | | | | | | | -3.337 | 1.00 28.01 |
| ATOM | 5217 | CB | LEU | 763 | -19.971 | 4.340 | | |
| MOTA | 5218 | CG | LEU | 763 | -19.364 | 2.960 | -3.070 | 1.00 30.99 |
| MOTA | 5219 | | LEU | 763 | -18.850 | 2.357 | -4.373 | 1.00 31.68 |
| MOTA | 5220 | | LEU | 763 | -18.224 | 3.087 | -2.071 | 1.00 30.71 |
| MOTA | 5221 | С | LEU | 763 | -20.602 | 6.576 | -2.416 | 1.00 24.34 |
| MOTA | 5222 | 0 | LEU | 763 | -19.725 | 7.319 | -1.974 | 1.00 20.25 |
| MOTA | 5223 | N | LEU | 764 | -21.616 | 7.013 | -3.154 | 1.00 24.14 |
| MOTA | 5224 | CA | LEU | 764 | -21.761 | 8.424 | -3.488 | 1.00 24.45 |
| MOTA | 5225 | CB | LEU | 764 | -22.988 | 8.633 | -4.380 | 1.00 24.40 |
| ATOM | 5226 | CG | LEU | 764 | -22.910 | 9.711 | -5.461 | 1.00 26.78 |
| ATOM | 5227 | | LEU | 764 | -24.307 | 9.955 | -6.006 | 1.00 27.16 |
| ATOM | 5228 | | LEU | 764 | -22.323 | 10.988 | -4.906 | 1.00 26.33 |
| | 5229 | C | LEU | 764 | -21.926 | 9.216 | -2.192 | 1.00 22.36 |
| ATOM | | | | | -21.257 | | | 1.00 22.30 |
| ATOM | 5230 | 0 | LEU | 764 | | 10.225 | -1.978 | |
| MOTA | 5231 | N | SER | 765 | -22.823 | 8.748 | -1.330 | 1.00 22.67 |
| MOTA | 5232 | CA | SER | 765 | -23.064 | 9.415 | -0.055 | 1.00 21.77 |
| MOTA | 5233 | CB | SER | 765 | -24.134 | 8.676 | 0.745 | 1.00 21.69 |
| MOTA | 5234 | OG | SER | 765 | -24.403 | 9.355 | 1.955 | 1.00 24.43 |
| MOTA | 5235 | С | SER | 765 | -21.779 | 9.486 | 0.766 | 1.00 20.68 |
| ATOM | 5236 | 0 | SER | 765 | -21.459 | 10.527 | 1.337 | 1.00 18.30 |
| ATOM | 5237 | N | ASP | 766 | -21.050 | 8.373 | 0.832 | 1.00 19.16 |
| ATOM | 5238 | CA | ASP | 766 | -19.801 | 8.338 | 1.585 | 1.00 19.55 |
| ATOM | 5239 | СВ | ASP | 766 | -19.213 | 6.917 | 1.623 | 1.00 19.61 |
| ATOM | 5240 | - | ASP | 766 | -19.907 | 6.011 | 2.643 | 1.00 23.80 |
| ATOM | 5241 | | ASP | 766 | -20.473 | 6.524 | 3.632 | 1.00 20.16 |
| ATOM | 5241 | | ASP | 766 | -19.863 | 4.774 | 2.458 | 1.00 24.88 |
| | | | | | | | | |
| ATOM | 5243 | С | ASP | 766 766 | -18.768 | 9.295 9.998 | 0.993 1.727 | 1.00 17.74 1.00 17.68 |
| ATOM | 5244 | 0 | ASP | 766 | -18.074 | | | |
| ATOM | 5245 | N | ALA | 767 | -18.666 | 9.321 | -0.332 | 1.00 18.82 |
| ATOM | 5246 | CA | ALA | 767 | -17.708 | 10.200 | -0.993 | 1.00 18.71 |
| ATOM | 5247 | CB | ALA | 767 | -17.759 | 9.992 | -2.501 | 1.00 18.07 |
| MOTA | 5248 | С | ALA | 767 | -17.992 | 11.658 | -0.647 | 1.00 18.35 |
| ATOM | 5249 | .0 | ALA | 767 | -17.081 | 12.408 | -0.289 | 1.00 17.25 |
| MOTA | 5250 | N | LEU | 768 | | 12.052 | -0.745 | 1.00 18.76 |
| ATOM | 5251 | CA | LEU | 768 | -19.674 | 13.421 | -0.437 | 1.00 18.68 |
| MOTA | 5252 | CB | LEU | 768 | -21.150 | 13.617 | -0.796 | 1.00 19.27 |
| MOTA | 5253 | CG | LEU | 768 | -21.490 | 13.710 | -2.291 | 1.00 19.38 |
| ATOM | 5254 | | LEU | 768 | -22.991 | 13.710 | -2.498 | |
| ATOM | 5255 | | LEU | 768 | -21.036 | 15.068 | -2.823 | 1.00 21.35 |
| | | | | | | | | |
| ATOM | 5256 | С | LEU | 768 | -19.465 | 13.744 | 1.033 | 1.00 18.16 |
| ATOM | 5257 | 0 | LEU | 768 | -19.127 | 14.878 | 1.392 | 1.00 18.53 |
| MOTA | 5258 | N | ALA | 769 | -19.669 | 12.746 | 1.886 | 1.00 15.98 |
| MOTA | 5259 | CA | ALA | 769 | -19.502 | 12.936 | 3.319 | 1.00 15.17 |
| MOTA | 5260 | CB | ALA | 769 | -20.038 | 11.726 | 4.069 | 1.00 17.07 |
| MOTA | 5261 | С | ALA | 769 | -18.033 | 13.166 | 3.661 | 1.00 14.89 |
| ATOM | E262 | 0 | ALA | 769 | -17.714 | 13.986 | 4.519 | 1.00 16.01 |
| | 5262 | 0 | | | | | | |
| ATOM | 5263 | N | LEU | 770 | -17.146 | 12.445 | 2.979 | 1.00 13.79 |
| ATOM ATOM | | | | | -17.146 -15.710 | 12.445 12.577 | 2.979 3.211 | 1.00 13.79 1.00 14.28 |

| ATOM | 5265 | СВ | LEU | 770 | -14.947 | 11.464 | 2.482 | 1.00 13.69 |
|--------------|--------------|----------|------------|------------|--------------------|------------------|------------------|--------------------------|
| ATOM | 5266 | CG | LEU | 770 | -15.159 | 10.031 | 3.022 | 1.00 14.90 |
| ATOM | 5267 | CD1 | LEU | 770 | -14.652 | 8.989 | 2.028 | 1.00 14.19 |
| ATOM | 5268 | | LEU | 770 | -14.439 | 9.898 | 4.346 | 1.00 14.20 |
| ATOM | 5269 | С | LEU | 770 | -15.250 | 13.940 | 2.713 | 1.00 14.23 |
| MOTA | 5270 | 0 | LEU | 770 | -14.387 | 14.585 | 3.319 | 1.00 15.29 |
| ATOM | 5271 | N | GLU | 771 771 | -15.826 -15.457 | 14.385 15.685 | 1.601 1.049 | 1.00 15.62 1.00 14.95 |
| ATOM ATOM | 5272 5273 | CA CB | GLU GLU | 771 | -16.126 | 15.892 | -0.311 | 1.00 14.93 |
| ATOM | 5274 | CG | GLU | 771 | -15.885 | 17.276 | -0.887 | 1.00 14.20 |
| ATOM | 5275 | CD | GLU | 771 | -16.600 | 17.471 | -2.201 | 1.00 16.87 |
| MOTA | 5276 | OE1 | | 771 | -17.837 | 17.270 | -2.243 | 1.00 16.35 |
| MOTA | 5277 | OE2 | GLU | 771 | -15.931 | 17.824 | -3.184 | 1.00 16.38 |
| ATOM | 5278 | С | GLU | 771 | -15.874 | 16.793 | 2.015 | 1.00 15.89 |
| ATOM | 5279 | 0 | GLU | 771 | -15.097 | 17.714 | 2.301 | 1.00 15.83 |
| ATOM | 5280 | N | ALA | 772 | -17.104 -17.653 | 16.696 17.677 | 2.512 3.449 | 1.00 15.87 1.00 17.16 |
| ATOM ATOM | 5281 5282 | CA CB | ALA ALA | 772 772 | -17.653 | 17.384 | 3.695 | 1.00 17.18 |
| ATOM | 5283 | C | ALA | 772 | -16.896 | 17.678 | 4.776 | 1.00 18.66 |
| ATOM | 5284 | ō | ALA | 772 | -16.855 | 18.695 | 5.472 | 1.00 17.21 |
| ATOM | 5285 | N | ALA | 773 | -16.294 | 16.537 | 5.115 | 1.00 18.43 |
| ATOM | 5286 | CA | ALA | 773 | -15.536 | 16.392 | 6.358 | 1.00 18.51 |
| MOTA | 5287 | CB | ALA | 773 | -15.359 | 14.909 | 6.690 | 1.00 17.94 |
| ATOM | 5288 | C | ALA | 773 | -14.170 | 17.067 | 6.265 | 1.00 17.57 |
| ATOM | 5289 | 0 | ALA | 773 774 | -13.539 -13.714 | 17.358 17.309 | 7.284 5.040 | 1.00 19.73 1.00 18.75 |
| ATOM ATOM | 5290 5291 | N CA | GLY GLY | 774 | -13.714 | 17.954 | 4.853 | 1.00 16.12 |
| ATOM | 5292 | C | GLY | 774 | -11.451 | 17.251 | 3.913 | 1.00 15.01 |
| ATOM | 5293 | ō | GLY | 774 | -10.395 | 17.797 | 3.600 | 1.00 13.07 |
| ATOM | 5294 | N | ALA | 775 | -11.786 | 16.048 | 3.451 | 1.00 15.01 |
| ATOM | 5295 | CA | ALA | 775 | -10.893 | 15.326 | 2.546 | 1.00 15.38 |
| MOTA | 5296 | CB | ALA | 775 | -11.513 | 13.990 | 2.134 | 1.00 15.63 |
| ATOM | 5297 | C | ALA | 775 | -10.610 | 16.171 | 1.308 | 1.00 15.18 |
| ATOM | 5298 5299 | O N | ALA GLN | 775 776 | -11.534 -9.337 | 16.705 16.270 | 0.708 0.924 | 1.00 14.76 1.00 14.50 |
| ATOM ATOM | 5300 | CA | GLN | 776 | -8.934 | 17.071 | -0.230 | 1.00 15.43 |
| ATOM | 5301 | CB | GLN | 776 | -7.695 | 17.893 | 0.129 | 1.00 15.10 |
| ATOM | 5302 | CG | GLN | 776 | -7.928 | 18.846 | 1.283 | 1.00 18.62 |
| ATOM | 5303 | CD | GLN | 776 | -6.658 | 19.513 | 1.747 | 1.00 18.59 |
| ATOM | 5304 | | GLN | 776 | -6.002 | 20.221 | 0.984 | 1.00 24.99 |
| ATOM | 5305 | NE2 | | 776 | -6.305 | 19.298 | 3.007 | 1.00 21.94 |
| ATOM | 5306 | C | GLN | 776 776 | -8.657 -8.344 | 16.233 16.765 | -1.474 -2.537 | 1.00 15.17 1.00 14.62 |
| ATOM ATOM | 5307 5308 | O N | GLN LEU | 777 777 | -8.767 | 14.918 | -1.330 | 1.00 14.02 |
| ATOM | 5309 | CA. | LEU | 777 | -8.547 | 13.990 | -2.429 | 1.00 15.20 |
| ATOM | 5310 | СВ | LEU | 777 | -7.057 | 13.673 | -2.562 | 1.00 16.16 |
| ATOM | 5311 | CG | LEU | 777 | -6.264 | 14.319 | -3.689 | 1.00 22.07 |
| ATOM | 5312 | | LEU | 777 | -4.776 | 13.947 | -3.529 | 1.00 20.46 |
| ATOM | 5313 | | | 777 | -6.792 | 13.831 | -5.042 | 1.00 23.78 |
| ATOM | 5314 | C | LEU | 777 | -9.316 | 12.710 | -2.125 | 1.00 15.07 |
| ATOM ATOM | 5315 5316 | O N | LEU LEU | 777 778 | -9.600 -9.654 | 12.419 11.954 | -0.966 -3.163 | 1.00 12.13 1.00 13.83 |
| ATOM | 5317 | CA | LEU | 778 | -10.375 | 10.701 | -2.979 | 1.00 14.56 |
| ATOM | 5318 | СВ | LEU | 778 | -11.891 | 10.887 | -3.176 | 1.00 14.01 |
| ATOM | 5319 | CG | LEU | 778 | -12.722 | 9.593 | -3.192 | 1.00 14.97 |
| MOTA | 5320 | | LEU | 778 | -12.716 | 8.948 | -1.806 | 1.00 15.87 |
| MOTA | 5321 | | LEU | 778 | -14.150 | 9.893 | -3.609 | 1.00 13.98 |
| ATOM | 5322 | C | LEU | 778 | -9.892 | 9.647 | -3.955 | 1.00 15.86 |
| ATOM | 5323 | 0 | LEU | 778 779 | -9.731 -9.639 | 9.913 8.450 | -5.150 -3.440 | 1.00 16.74 1.00 14.91 |
| MOTA MOTA | 5324 5325 | N CA | VAL VAL | 779 | -9.039 -9.235 | 7.348 | -4.295 | 1.00 15.20 |
| ATOM | 5326 | CB | VAL | 779 | -8.057 | 6.528 | -3.694 | 1.00 15.02 |
| ATOM | 5327 | CG1 | | 779 | -7.850 | 5.242 | -4.509 | 1.00 14.33 |
| ATOM | 5328 | | VAL | 779 | -6.774 | 7.354 | -3.730 | 1.00 15.87 |
| ATOM | 5329 | С | VAL | 779 | -10.465 | 6.453 | -4.416 | 1.00 15.26 |
| MOŢA | 5330 | 0 | VAL | 779 | -11.171 | 6.222 | -3.430 | 1.00 14.26 |
| MOTA | 5331 | N | LEU | 780 | -10.725 | 5.982 | -5.632 | 1.00 16.87 |
| ATOM | 5332 | CA | LEU | 780 780 | -11.854 -12.807 | 5.094 5.737 | -5.928 -6.937 | 1.00 18.23 1.00 20.90 |
| ATOM ATOM | 5333 5334 | CB CG | LEU LEU | 780 780 | -12.807 -14.160 | 6.196 | -6.413 | 1.00 20.90 |
| ATOM | 5335 | | LEU | 780 | -15.027 | 6.667 | -7.586 | 1.00 22.61 |
| ATOM | 5336 | | LEU | 780 | -14.841 | 5.046 | -5.677 | 1.00 24.16 |
| ATOM | 5337 | С | LEU | 780 | -11.263 | 3.841 | -6.535 | 1.00 17.70 |
| ATOM | 5338 | 0 | LEU | 780 | -10.617 | 3.912 | -7.580 | 1.00 18.28 |
| ATOM | 5339 | N | GLU | 781 | -11.485 | 2.693 | -5.895 | 1.00 17.11 |
| ATOM ATOM | 5340 5341 | CA | GLU | 781 781 | -10.913 -9.972 | 1.434 0.857 | -6.386 -5.314 | 1.00 18.49 1.00 19.29 |
| 22 OF1 | 22#I | СВ | GLU | ,01 | 2.312 | 0.057 | J.J.4 | 2.00 17.29 |

```
5342
             CG
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ATOM
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                         781
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ATOM
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ATOM
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ATOM
       5393
              CA
                  ALA
                         788
ATOM
       5394
              CB
                  ALA
                         788
                                  -15.794
                                             5.843 -11.564
                                                             1.00 21.55
                                            7.817 -11.510
ATOM
       5395
                  ALA
                         788
                                  -17.337
                                                             1.00 23.99
              C
                                            8.855 -11.020
ATOM
       5396
              0
                  ALA
                         788
                                  -16.890
                                                             1.00 23.15
       5397
                         789
                                  -18.117
                                            7.808 -12.586
                                                             1.00 25.42
ATOM
              Ν
                  LYS
                                                             1.00 25.60
ATOM
       5398
              CA
                  LYS
                         789
                                  -18.495
                                             9.050 -13.254
       5399
              CB
                         789
                                  -19.273
                                            8.758 -14.537
                                                             1.00 29.58
ATOM
                  LYS
                                            7.660 -15.392
       5400
                         789
                                 -18.679
                                                             1.00 34.03
ATOM
              CG
                  LYS
                                            7.537 -16.722
ATOM
       5401
              CD
                  LYS
                         789
                                 -19.410
                                                             1.00 37.45
       5402
                         789
                                  -18.909
                                             6.342 -17.513
                                                             1.00 37.98
ATOM
              CE
                  LYS
ATOM
       5403
             NZ
                  LYS
                         789
                                  -19.397
                                            6.370 -18.912
                                                             1.00 39.55
                                            9.883 -12.323
                                                             1.00 24.36
                         789
                                 -19.365
ATOM
       5404
                  LYS
              С
                                           11.074 -12.140
ATOM
       5405
              0
                  LYS
                         789
                                 -19.124
                                                            1.00 23.55
ATOM
       5406
              N
                  ARG
                         790
                                  -20.380
                                            9.254 -11.737
                                                             1.00 23.75
ATOM
       5407
              CA
                  ARG
                         790
                                  -21.275
                                             9.959 -10.824
                                                             1.00 23.75
              CB
                         790
                                  -22.320
                                            9.011 -10.229
                                                             1.00 26.20
ATOM
       5408
                  ARG
                                            8.564 -11.192
                                                             1.00 31.43
                         790
                                 -23.400
ATOM
       5409
              CG
                  ARG
ATOM
       5410
              CD
                  ARG
                         790
                                 -24.747
                                            8.502 -10.483
                                                             1.00 34.23
                         790
                                  -24.766
                                            7.564
                                                    -9.362
                                                             1.00 33.07
ATOM
       5411
             NE
                  ARG
ATOM
       5412
                         790
                                  -25.553
                                            7.694
                                                    -8.297
                                                             1.00 35.30
              CZ
                  ARG
                                            8.725
                                                             1.00 37.31
ATOM
                         790
                                                    -8.205
       5413
              NH1
                  ARG
                                  -26.380
ATOM
       5414
             NH2
                  ARG
                         790
                                  -25.525
                                            6.793
                                                    -7.323
                                                             1.00 35.56
ATOM
       5415
                  ARG
                         790
                                  -20.510
                                           10.612
                                                    -9.680
                                                             1.00 22.42
              C
ATOM
       5416
              0
                  ARG
                         790
                                  -20.752
                                           11.767
                                                    -9.329
                                                             1.00 20.30
ATOM
                         791
                                  -19.584
                                            9.864
                                                    -9.098
                                                             1.00 20.17
       5417
              N
                  ILE
                                                    -7.979
                                                             1.00 18.67
```

ATOM

5418

CA

ILE

791

-18.811

10.374

| ATOM | 5419 | СВ | ILE | 791 | -17.999 | 9.232 | -7.310 | 1.00 | 18.12 |
|--------------|--------------|------------|------------|--------------|--------------------|------------------|--------------------|------|----------------|
| ATOM | 5420 | CG2 | ILE | 791 | -16.996 | 9.802 | -6.317 | 1.00 | 16.97 |
| ATOM | 5421 | CG1 | ILE | 791 | -18.971 | 8.276 | -6.599 | 1.00 | 20.08 |
| ATOM | 5422 | CD1 | ILE | 791 | -18.299 | 7.133 | -5.849 | 1.00 | 23.20 |
| ATOM | 5423 | С | ILE | 791 | -17.883 | 11.504 | -8.402 | | 15.86 |
| MOTA | 5424 | 0 | ILE | 791 | -17.806 | 12.533 | -7.732 | | 15.97 |
| ATOM | 5425 | N | THR | 792 | -17.192 | 11.315 | -9.519 | 1.00 | 17.74 |
| ATOM | 5426 | CA | THR | 792 | -16.271 | | -10.014 | | 19.29 |
| ATOM | 5427 | CB | THR | 792 | -15.511 | | -11.242 | | 19.17 |
| ATOM | 5428 | · 0G1 | THR THR | 792 792 | -14.779 -14.539 | | -10.890 -11.737 | 1.00 | 17.58 18.00 |
| ATOM ATOM | 5429 5430 | CGZ | THR | 792 | -17.004 | | -10.360 | | 20.60 |
| ATOM | 5431 | 0 | THR | 792 | -16.476 | | -10.300 | | 20.78 |
| ATOM | 5432 | N | GLU | 793 | -18.216 | | -10.891 | | 20.13 |
| ATOM | 5433 | CA | GLU | 793 | -18.971 | | -11.236 | | 21.99 |
| ATOM | 5434 | CB | GLU | 793 | -20.014 | 14.392 | -12.307 | 1.00 | 24.27 |
| MOTA | 5435 | CG | GLU | 793 | -19.412 | | -13.589 | | 27.80 |
| MOTA | 5436 | CD | GLU | 793 | -20.427 | | -14.703 | | 31.99 |
| MOTA | 5437 | | GLU | 793 | -21.513 | | -14.477 | | 33.12 |
| MOTA | 5438 | OE2 | | 793 | -20.135 | | -15.808 | | 34.84 |
| ATOM | 5439 | С | GLU | 793 | -19.654 -19.869 | | -10.023 -9.990 | | 21.66 22.52 |
| ATOM ATOM | 5440 5441 | O N | GLU ALA | 793 794 | -19.869 | 16.546 14.528 | -9.990 | | 20.04 |
| ATOM | 5442 | CA | ALA | 794 | -20.648 | 15.054 | -7.832 | | 19.93 |
| ATOM | 5443 | CB | ALA | 794 | -21.394 | 13.936 | -7.102 | | 21.36 |
| ATOM | 5444 | c | ALA | 794 | -19.679 | 15.739 | -6.868 | | 20.03 |
| MOTA | 5445 | 0 | ALA | 794 | -20.088 | 16.572 | -6.064 | 1.00 | 20.59 |
| ATOM | 5446 | N | LEU | 795 | -18.399 | 15.396 | -6.940 | 1.00 | 19.04 |
| MOTA | 5447 | CA | LEU ' | 795 | -17.424 | 15.990 | -6.034 | | 17.59 |
| MOTA | 5448 | CB | LEU | 795 | -16.488 | 14.910 | -5.483 | | 20.28 |
| MOTA | 5449 | CG | LEU | 795 | -17.098 | 13.760 | -4.674 | | 23.20 |
| MOTA | 5450 | | LEU | 795 | -15.962 | 12.889 | -4.142 | | 22.33 |
| ATOM | 5451 | | LEU | 795 795 | -17.934 -16.586 | 14.285 | -3.527 -6.657 | | 26.37 15.79 |
| MOTA MOTA | 5452 5453 | C 0 | LEU LEU | 795 795 | -16.268 | 17.098 17.065 | -7.846 | | 16.54 |
| ATOM | 5454 | N | | . 796 | -16.227 | 18.082 | -5.840 | 1.00 | 15.08 |
| ATOM | 5455 | CA | ALA | 796 | -15.404 | 19.185 | -6.310 | 1.00 | 15.70 |
| ATOM | 5456 | CB | | 796 | -15.684 | 20.435 | -5.494 | 1.00 | 15.40 |
| ATOM | 5457 | С | ALA | 796 | ~13.936 | 18.789 | -6.193 | 1.00 | 14.51 |
| MOTA | 5458 | 0 | ALA | 796 | -13.108 | 19.193 | -7.008 | 1.00 | 13.29 |
| MOTA | 5459 | N | ILE | 797 | -13.617 | 17.989 | -5.175 | | 14.50 |
| ATOM | 5460 | CA | ILE | 797 | -12.243 | 17.546 | -4.972 | 1.00 | 13.86 |
| MOTA | 5461 | CB | ILE | 797 | -12.029 | 16.916 | -3.560 | 1.00 | 14.10 |
| MOTA MOTA | 5462 5463 | CG2 CG1 | | 797 797 | -12.315 -12.932 | 17.932 15.694 | -2.488 -3.365 | 1.00 | 13.02 15.07 |
| ATOM | 5464 | | ILE | 797 | -12.592 | 14.909 | -2.090 | 1.00 | 16.44 |
| MOTA | 5465 | C | ILE. | 797 | -11.862 | 16.526 | -6.034 | | 12.69 |
| ATOM | 5466 | Ō | ILE | 797 | -12.720 | 15.843 | -6.595 | 1.00 | 14.87 |
| ATOM | 5467 | N | PRO | 798 | -10.565 | 16.419 | -6.340 | 1.00 | 14.26 |
| ATOM | 5468 | CD | PRO | 798 | -9.444 | 17.299 | -5.974 | 1.00 | 15.87 |
| MOTA | 5469 | CA | PRO | 798 | -10.181 | 15.446 | -7.359 | | 13.35 |
| MOTA | 5470 | CB | PRO | 798 | -8.720 | 15.796 | | | 15.01 |
| MOTA | 5471 | CG | PRO | 798 | -8.256 | 16.532 | -6,455 | | 18.28 |
| ATOM ATOM | 5472 5473 | C O | PRO PRO | 798 798 | -10.377 -10.202 | 14.004 13.665 | -6.920 -5.745 | 1.00 | 13.85 12.45 |
| ATOM | 5474 | N | VAL | 799 | -10.764 | 13.169 | -7.879 | 1.00 | 13.99 |
| ATOM | 5475 | CA | VAL | 799 | -10.992 | 11.750 | -7.633 | 1.00 | 15.13 |
| ATOM | 5476 | CB | VAL | 799 | -12.432 | 11.349 | -8.019 | | 16.02 |
| MOTA | 5477 | | VAL | 799 | -12.605 | 9.845 | -7.864 | 1.00 | 14.52 |
| ATOM | 5478 | CG2 | VAL | 799 | -13.422 | 12.080 | -7.119 | 1.00 | 14.06 |
| MOTA | 5479 | C | VAL | 799 | -9.994 | 10.941 | -8.439 | 1.00 | 14.87 |
| MOTA | 5480 | 0 | VAL | 799 | -9.949 | 11.029 | -9.663 | | 15.59 |
| ATOM | 5481 | N | ILE | 800 | -9.186 | 10.162 | -7.731 | 1.00 | 14.30 |
| ATOM | 5482 5483 | CA | ILE ILE | 800 | -8.170 | 9.335 9.375 | -8.350 -7.528 | | 14.45 15.69 |
| ATOM | 5484 | CB | ILE | 800 800 | -6.861 -5.830 | 8.414 | -8.128 | | 14.51 |
| ATOM ATOM | 5485 | | ILE | 800 | -6.315 | 10.810 | -7.524 | 1.00 | 15.10 |
| ATOM | 5486 | | ILE | 800 | -5.074 | 11.021 | -6.676 | | 17.30 |
| ATOM | 5487 | c | ILE | 800 | -8.691 | 7.911 | -8.429 | 1.00 | 14.61 |
| ATOM | 5488 | 0 | ILE | 800 | -9.113 | 7.334 | -7.424 | | 13.66 |
| MOTA | 5489 | N | GLY | 801 | -8.672 | 7.349 | -9.629 | | 13.09 |
| MOTA | 5490 | CA | GLY | 801 | -9.178 | 6.005 | -9.783 | 1.00 | 12.12 |
| MOTA | 5491 | С | GLY | 801 | -8.151 | | -10.061 | 1.00 | 13.23 |
| ATOM | 5492 | 0 | GLY | 801 | -7.055 · | | -10.549 | | 12.71 |
| ATOM | 5493 | N | ILE | 802 802 | -8.522 -7.712 | 3.713 2.533 | -9.703 -9.954 | 1.00 | 14.81 16.00 |
| ATOM ATOM | 5494 5495 | CA CB | ILE | 802 · 802 | -7.712 -6.799 | 2.333 | -8.739 | | 15.76 ^ |
| | | | | | | | | | |

| ATOM | 5496 | CG2 | ILE | 802 | -7.575 | 2.202 -7.439 | 1.00 18.40 |
|------|--------------|-----------|------|------|---------|----------------|------------|
| ATOM | 5497 | CG1 | ILE | 802 | -6.172 | 0.792 -8.967 | 1.00 20.03 |
| ATOM | 5498 | CD1 | ILE | 802 | -5.323 | 0.706 -10.195 | 1.00 20.86 |
| ATOM | 5499 | С | ILE | 802 | -8.773 | 1.468 -10.223 | 1.00 15.80 |
| ATOM | 5500 | ō | ILE | 802 | -9.548 | 1.112 -9.343 | 1.00 16.52 |
| ATOM | 5501 | N | GLY | 803 | -8.831 | 1.008 -11.466 | 1.00 18.14 |
| ATOM | 5502 | CA | GLY | 803 | -9.826 | 0.024 -11.834 | 1.00 18.81 |
| ATOM | 5502 | C | GLY | 803 | -11.211 | 0.649 -11.819 | 1.00 19.32 |
| ATOM | 5504 | 0 | GLY | 803 | -12.206 | -0.041 -11.600 | 1.00 20.70 |
| | 5505 | | ALA | 804 | -11.278 | 1.957 -12.049 | 1.00 20.70 |
| ATOM | | N | | | | 2.676 -12.049 | 1.00 17.72 |
| ATOM | 5506 | CA | ALA | 804 | -12.544 | | |
| ATOM | 5507 | CB | ALA | 804 | -12.547 | 3.719 -10.922 | 1.00 16.05 |
| ATOM | 5508 | C | ALA | 804 | -12.834 | 3.359 -13.382 | 1.00 17.22 |
| ATOM | 5509 | 0 | ALA | 804 | -13.727 | 4.205 -13.478 | 1.00 19.29 |
| MOTA | 5510 | N | GLY | 805 | -12.079 | 2.999 -14.412 | 1.00 17.74 |
| MOTA | 5511 | CA | GLY | 805 | -12.289 | 3.595 -15.718 | 1.00 19.47 |
| MOTA | 5512 | С | GLY | 805 | -11.524 | 4.893 -15.885 | 1.00 19.16 |
| MOTA | 5513 | 0 | GLY | 805 | -10.832 | 5.336 -14.964 | 1.00 19.03 |
| MOTA | 5514 | N | ASN | 806 | -11.646 | 5.509 -17.057 | 1.00 17.88 |
| ATOM | 5515 | CA | ASN | 806 | -10.939 | 6.760 -17.324 | 1.00 18.23 |
| MOTA | 5516 | CB | ASN | 806 | -10.410 | 6.784 -18.769 | 1.00 16.49 |
| ATOM | 5517 | CG | ASN | 806 | -11.511 | 6.953 -19.810 | 1.00 18.05 |
| MOTA | 5518 | OD1 | ASN | 806 | -11.225 | 7.247 -20.972 | 1.00 19.59 |
| ATOM | 5519 | ND2 | ASN | 806 | -12.767 | 6.760 -19.404 | 1.00 12.05 |
| ATOM | 5520 | С | ASN | 806 | -11.774 | 8.006 -17.062 | 1.00 18.00 |
| ATOM | 5521 | 0 | ASN | 806 | -11.411 | 9.091 -17.497 | 1.00 18.99 |
| ATOM | 5522 | N | VAL | 807 | -12.872 | 7.848 -16.331 | 1.00 17.63 |
| ATOM | 5523 | CA | VAL | 807 | -13.756 | 8.965 -16.033 | 1.00 19.39 |
| ATOM | 5524 | СВ | VAL | 807 | -15.205 | 8.489 -15.860 | 1.00 21.52 |
| ATOM | 5525 | | VAL | 807 | -16.140 | 9.685 -15.847 | 1.00 27.73 |
| ATOM | 5526 | CG2 | VAL | 807 | -15.578 | 7.547 -16.990 | 1.00 24.38 |
| ATOM | 5527 | C | VAL | 80.7 | -13.354 | 9.738 -14.783 | 1.00 18.27 |
| MOTA | 5528 | o | VAL | 807 | -13.941 | 10.770 -14.478 | 1.00 16.18 |
| ATOM | 5529 | N | THR | 808 | -12.361 | 9.237 -14.057 | 1.00 18.22 |
| | 5530 | CA | THR | 808 | -11.899 | 9.915 -12.854 | 1.00 14.60 |
| MOTA | | | | | | | |
| ATOM | 5531 | CB | THR | 808 | -11.203 | 8.920 -11.885 | |
| ATOM | 5532 | OG1 | THR | 808 | -10.153 | 8.222 -12.567 | 1.00 14.17 |
| MOTA | 5533 | CG2 | THR | 808 | -12.215 | 7.923 -11.346 | 1.00 12.82 |
| ATOM | 5534 | C | THR | 808 | -10.944 | 11.044 -13.250 | 1.00 16.13 |
| MOTA | 5535 | 0 | THR | 808 | -10.476 | 11.103 -14.390 | 1.00 16.23 |
| MOTA | 5536 | N | ASP | 809 | -10.675 | 11.948 -12.312 | 1.00 15.76 |
| MOTA | 5537 | CA | ASP | 809 | -9.790 | 13.086 -12.556 | 1.00 15.32 |
| MOTA | 5538 | CB | AȘP | 809 | -9.912 | 14.095 -11.405 | 1.00 14.96 |
| ATOM | 5539 | CG | ASP. | 809 | -11.332 | 14.591 -11.221 | 1.00 15.54 |
| MOTA | 5540 | | ASP | 809 | -11.890 | 15.153 -12.191 | 1.00 17.46 |
| ATOM | 5541 | | ASP | 809 | -11.897 | 14.428 -10.126 | 1.00 17.01 |
| MOTA | . 5542 | C | ASP | 809 | -8.342 | 12.633 -12.691 | 1.00 15.52 |
| MOTA | 5543 | 0 | ASP | 809 | -7.535 | 13.266 -13.379 | 1.00 14.60 |
| ATOM | 5544 | N | GLY | 810 | -8.021 | 11.528 -12.031 | 1.00 15.18 |
| MOTA | 5545 | CA | GLY | 810 | -6.673 | 11.011 -12.089 | 1.00 15.09 |
| MOTA | 5546 | С | GLY | 810 | -6.630 | 9.501 -12.037 | 1.00 14.54 |
| MOTA | 5547 | 0 | GLY | 810 | -7.656 | 8.831 -11.914 | 1.00 14.65 |
| ATOM | 5548 | N | GLN | 811 | -5.424 | 8.964 -12.115 | 1.00 14.84 |
| MOTA | 5549 | CA | GLN | 811 | -5.242 | 7.528 -12.093 | 1.00 14.60 |
| MOTA | 5550 | CB | GLN | 811 | -4.929 | 7.035 -13.506 | 1,00 15.54 |
| MOTA | 5551 | CG | GLN | 811 | -6.026 | 7.268 -14.523 | 1.00 16.05 |
| ATOM | 5552 | CD | GLN | 811 | -7.254 | 6.423 -14.248 | 1.00 14.86 |
| ATOM | 5553 | OE1 | GLN | 811 | -7.145 | 5.274 -13.812 | 1.00 15.67 |
| ATOM | 5554 | NE2 | | 811 | -8.428 | 6.982 -14.513 | 1.00 13.00 |
| ATOM | 5555 | C | GLN | 811 | -4.095 | 7.146 -11.173 | 1.00 16.44 |
| MOTA | 5556 | 0 | GLN | 811 | -3.179 | 7.933 -10.940 | 1.00 12.57 |
| ATOM | 5557 | N | ILE | 812 | -4.151 | 5.932 -10.648 | 1.00 18.01 |
| ATOM | 5558 | CA | ILE | 812 | -3.080 | 5.448 -9.795 | 1.00 21.55 |
| MOTA | 5559 | CB | ILE | 812 | -3.394 | 5.680 -8.286 | 1.00 22.97 |
| ATOM | 5560 | CG2 | ILE | 812 | -4.477 | 4.732 -7.810 | 1.00 24.22 |
| ATOM | 5561 | CG1 | ILE | | -2.116 | 5.495 -7.461 | 1.00 26.66 |
| ATOM | 5562 | CD1 | ILE | 812 | -2.168 | 6.141 -6.077 | 1.00 27.37 |
| ATOM | 5563 | CDI | ILE | 812 | -2.880 | 3.968 -10.098 | 1.00 23.39 |
| ATOM | 5564 | .0 | ILE | 812 | -3.781 | 3.292 -10.599 | 1.00 22.15 |
| ATOM | 5565 | Ŋ | LEU | 813 | -1.678 | 3.478 -9.832 | 1.00 25.42 |
| ATOM | 5566 | CA | LEU | 813 | -1.369 | 2.081 -10.072 | 1.00 27.98 |
| ATOM | | CB | | 813 | -1.231 | 1.814 -11.572 | 1.00 27.38 |
| | 5567 5569 | | LEU | | -2.228 | 0.842 -12.220 | 1.00 29.40 |
| ATOM | 5568 | CG CD1 | LEU | 813 | | | 1.00 35.93 |
| MOTA | 5569 | | LEU | 813 | -1.759 | 0.552 -13.636 | |
| ATOM | 5570 | | LEU | 813 | -2.306 | -0.460 -11.426 | 1.00 34.60 |
| ATOM | 5571 | C | LEU | 813 | -0.075 | 1.704 -9.375 | 1.00 27.36 |
| ATOM | 5572 | 0 | LEU | 813 | 0.783 | 2.558 -9.138 | 1.00 24.70 |
| | | | | | | | |

| ATOM | 5573 | N | VAL | 814 | 0.046 | 0.422 | -9.038 | 1.00 27.73 |
|--------------|--------------|------------|------------|------------|----------------|--------------------|--------------------|--------------------------|
| ATOM | 5574 | CA | VAL | 814 | 1.238 | -0.099 | -8.388 | 1.00 24.77 |
| MOTA | 5575 | CB | VAL | 814 | 0.992 | -1.504 | -7.775 | 1.00 26.98 |
| ATOM | 5576 | CG1 | VAL | 814 | 2.285 | -2.045 | -7.170 | 1.00 27.58 |
| ATOM | 5577 | CG2 | VAL | 814 | -0.088 | -1.420 | -6.705 | 1.00 29.29 |
| ATOM | 5578 | C | VAL | 814 | 2.313 | -0.208 | -9.456 | 1.00 21.90 |
| MOTA | 5579 | 0 | VAL | 814 | 2.128 | -0.851 | -10.487 | 1.00 19.33 |
| MOTA | 5580 | N | MET | 815 | 3.441 | 0.438 | -9.202 | 1.00 20.34 |
| ATOM | 5581 | CA | MET | 815 | 4.546 | 0.432 | -10.142 | 1.00 18.61 |
| MOTA | 5582 | CB | MET | 815 | 5.710 | 1.244 | -9.564 | 1.00 15.22 |
| MOTA | 5583 | CG | MET | 815 | 6.183 | 0.786 | -8.190 | 1.00 15.35 |
| MOTA | 5584 | SD | MET | 815 | 7.964 | 0.942 | -8.143 | 1.00 16.36 |
| MOTA | 5585 | CE | MET | 815 | 8.452 | -0.581 | -8.957 | 1.00 11.50 |
| ATOM | 5586 | С | MET | 815 | 5.020 | -0.973 | -10.521 | 1.00 17.74 |
| ATOM | 5587 | 0 | MET | 815 | 5.483 | -1.205 | -11.639 | 1.00 19.67 |
| ATOM | 5588 | N | HIS | 816 | 4.908 | -1.918 | -9.597 | 1.00 17.17 |
| ATOM | 5589 | CA | HIS | 816 | 5.358 | -3.276 | -9.870 | 1.00 17.66 |
| ATOM | 5590 | CB | HIS | 816 | 5.319 | -4.091 | -8.570 | 1.00 16.96 |
| MOTA | 5591 | CG | HIS | 816 | 6.334 | -3.639 | | 1.00 16.58 |
| MOTA | 5592 | CD2 | HIS | 816 | 6.312 | -2.620 | -6.675 | 1.00 14.97 |
| ATOM | 5593 | ND1 | HIS | 816 | 7.604 | -4.173 | -7.503 | 1.00 18.92 |
| MOTA | 5594 | CE1 | HIS | 816 | 8.322 | -3.500 | -6.622 | 1.00 15.55 |
| MOTA | 5595 | NE2 | HIS | 816 | 7.561 | -2.551 | -6.106 | 1.00 21.47 |
| MOTA | 5596 | C | HIS | 816 | 4.578 | -3.953 | -10.994 | 1.00 20.90 |
| MOTA | 5597 | 0 | HIS | 816 | 5.096 | -4.844 | -11.663 | 1.00 20.05 |
| MOTA | 5598 | N | ASP | 817 | 3.340 | -3.524 | -11.217 | 1.00 23.00 |
| MOTA | 5599 | CA | ASP | 817 | 2.526 | -4.095 | -12.294 | 1.00 25.53 |
| ATOM | 5600 | CB | ASP | 817 | 1.041 | -4.013 | -11.939 | 1.00 29.00 |
| MOTA | 5601 | CG | ASP | 817 | 0.689 | -4.830 | -10.710 | 1.00 32.54 |
| MOTA | 5602 | OD1 | ASP | 817 | 0.878 | -6.062 | -10.742 | 1.00 34.60 |
| MOTA | 5603 | OD2 | ASP | 817 | 0.224 | -4.234 | -9.716 | 1.00 34.24 |
| MOTA | 5604 | С | ASP | 817 · | 2.786 | -3.341 | -13.602 | 1.00 26.31 |
| ATOM | 5605 | 0 | ASP | 817 | 2.743 | -3.925 | -14.687 | 1.00 27.79 |
| MOTA | 5606 | N | ALA | 818 | 3.064 | -2,045 | -13.489 | 1.00 27.64 |
| MOTA | 5607 | CA | ALA | 818 | 3.330 | -1.195 | -14.651 | 1.00 27.51 |
| MOTA | 5608 | CB | ALA | 818 | 3.461 | 0.262 | -14.204 | 1.00 28.70 |
| ATOM | 5609 | С | ALA | 818 | 4.573 | | -15.438 | 1.00 28.22 |
| MOTA | 5610 | 0 | ALA | 818 | 4.661 | -1.348 | -16.640 | 1.00 27.43 |
| MOTA | 5611 | N | PHE | 819 | 5.536 | | -14.765 | 1.00 26.40 |
| MOTA | 5612 | CA | PHE | 819 | 6.764 | | -15.434 | 1.00 25.70 |
| MOTA | 5613 | CB | PHE | 819 | 7.994 | | -14.705 | 1.00 26.29 |
| MOTA | 5614 | CG | PHE | 819 | 7.889 | | -14.359 | 1.00 27.48 |
| MOTA | 5615 | | PHE | 819 | 7.412 | | -15.292 | 1.00 28.59 |
| MOTA | 5616 | | PHE | 819 | 8.248 | | -13.094 | 1.00 28.81 |
| MOTA | 5617 | | PHE | 819 | 7.289 | | -14.975 | 1.00 29.43 |
| MOTA | 5618 | | PHE | 819 | 8.131 | | -12.763 | 1.00 29.98 |
| ATOM | 5619 | CZ | PHE | 819 | 7.648 | | -13.707 | 1.00 30.70 |
| MOTA | 5620 | C | PHE | 819 | 6.869 | | -15.551 | 1.00 25.12 |
| ATOM | 5621 | Ο ΄ | PHE | 819 | 7.935 | | -15.846 | 1.00 24.68 |
| ATOM | 5622 | N | GLY | 820 | 5.753 | | -15.323 | 1.00 24.44 |
| ATOM | 5623 | CA | GLY | 820 | 5.738 | | -15.419 | 1.00 24.57 |
| MOTA | 5624 | C | GLY | 820 | 6.655 | | -14.429 | 1.00 25.69 |
| ATOM | 5625 | 0 | GLY | 820 | 7.124 | | -14.688 | 1.00 25.84 |
| MOTA | 5626 | N | ILE | 821 | 6.919 | | -13.297 | 1.00 23.27 |
| MOTA | 5627 | CA | ILE | 821 | 7.779 | | -12.277 | 1.00 22.14 |
| ATOM | 5628 | CB | ILE | 821 | 8.241 | | -11.247 | 1.00 20.40 |
| MOTA | 5629 | CG2 | ILE | 821 | 9.023 | | -10.110. | |
| ATOM | 5630 | CG1 | ILE | 821 | 9.099 | | -11.956 | 1.00 19.76 |
| MOTA | 5631 | CD1 | ILE | 821 | 9.420 | | -11.125 | 1.00 17.39 |
| ATOM | 5632 | , C | ILE | 821 | 7.015 | | -11.565 -11.342 | 1.00 22.87 1.00 21.66 |
| MOTA | 5633 5634 | 0 | ILE | 821 | 7.542 | | | 1.00 21.88 |
| ATOM | | N | THR | 822 | 5.757 | | -11.238 | |
| ATOM | 5635 | CA | THR | 822 | 4.916 | | -10.562 | 1.00 28.76 |
| ATOM | 5636 | CB OC1 | THR | 822 | 3.548 | | -10.196 -11.327 | 1.00 29.81 1.00 35.04 |
| ATOM ATOM | 5637 5638 | OG1 CG2 | THR THR | 822 822 | 3.020 3.697 | -7.441 -7.184 | -9.036 | 1.00 35.04 |
| ATOM | 5639 | .C | THR | 822 | 4.689 | -10.014 | | 1.00 29.32 |
| ATOM | 5640 | 0 | THR | 822 | 4.675 | • | -12.638 | 1.00 31.12 |
| ATOM | 5641 | N | GLY | 823 | | -11.142 | | 1.00 28.97 |
| | 5642 | CA | GLY | 823 | | -11.142 -12.431 | | 1.00 33.39 |
| ATOM ATOM | 5643 | CA | GLY | 823 | | -12.431 | | 1.00 39.65 |
| ATOM | 5644 | 0 | GLY | 823 | | -12.358 | | 1.00 45.12 |
| ATOM | 5645 | N | GLY | 824 | | -12.560 | | 1.00 45.19 |
| ATOM | 5646 | CA | GLY | 824 | | -12.584 | | 1.00 47.84 |
| ATOM | 5647 | C | GLY | 824 | | -12.505 | | 1.00 47.84 |
| MOTA | 5648 | 0 | GLY | 824 | | -12.463 | | 1.00 50.56 |
| ATOM | 5649 | N | HIS | 825 | | -12.481 | | 1.00 50.83 |
| | | | | • | | | | |

| MOTA | 5650 | CA | HIS | 825 | -1.077 | -12.408 | -14.248 | 1.00 52.44 |
|------|------|-----------|-----|-------|--------|---------|--------------------|------------|
| ATOM | 5651 | CB | HIS | 825 | -1.737 | -13.633 | -13.610 | 1.00 54.90 |
| ATOM | 5652 | CG | HIS | 825 | -1.153 | -14.935 | -14.063 | 1.00 57.95 |
| ATOM | 5653 | | HIS | 825 | | -15.900 | | 1.00 58.90 |
| ATOM | 5654 | | HIS | 825 | | -15.355 | | 1.00 59.02 |
| ATOM | 5655 | | HIS | 825 | | -16.522 | | 1.00 59.10 |
| | | | HIS | | | -16.874 | | 1.00 58.90 |
| ATOM | 5656 | | | 825 | | | | |
| ATOM | 5657 | С | HIS | 825 | | -11.131 | | 1.00 51.18 |
| ATOM | 5658 | 0 | HIS | 825 | | -11.188 | | 1.00 51.71 |
| MOTA | 5659 | N | ILE | 826 | -1.120 | | -14.055 | 1.00 50.05 |
| ATOM | 5660 | CA | ILE | 826 | -1.566 | -8.698 | -13.516 | 1.00 48.19 |
| ATOM | 5661 | CB | ILE | 826 | -0.883 | -7.510 | -14.230 | 1.00 48.89 |
| ATOM | 5662 | CG2 | ILE | 826 | 0.631 | -7.612 | -14.078 | 1.00 50.27 |
| ATOM | 5663 | CG1 | ILE | 826 | -1.280 | -7.484 | -15.707 | 1.00 49.07 |
| ATOM | 5664 | CD1 | | 826 | -0.762 | | -16.460 | 1.00 47.09 |
| ATOM | 5665 | C | ILE | 826 | -3.077 | | -13.640 | 1.00 46.15 |
| ATOM | 5666 | ō | ILE | 826 | -3.707 | | -14.520 | 1.00 45.71 |
| ATOM | 5667 | N | PRO | 827 | -3.678 | | -12.758 | 1.00 44.37 |
| | | | | | -3.037 | | -11.700 | 1.00 43.85 |
| ATOM | 5668 | CD | PRO | 827 | | | | |
| ATOM | 5669 | CA | PRO | 827 | -5.124 | | -12.780 | 1.00 43.13 |
| ATOM | 5670 | CB | PRO | 827 | -5.344 | | -11.560 | 1.00 44.15 |
| ATOM | 5671 | CG | PRO | 827 | -4.058 | | -11.457 | 1.00 45.19 |
| ATOM | 5672 | C | PRO | 827 | -5.625 | | -14.073 | 1.00 40.91 |
| MOTA | 5673 | 0 | PRO | 827 | -4.887 | | -14.753 | 1.00 40.25 |
| MOTA | 5674 | N | LYS | 828 | -6.884 | -7.116 | -14.402 | 1.00 39.31 |
| MOTA | 5675 | CA | LYS | 828 | -7.500 | -6.580 | -15.610 | 1.00 37.09 |
| ATOM | 5676 | CB | LYS | 828 | -8.976 | -6.986 | -15.682 | 1.00 40.38 |
| ATOM | 5677 | CG | LYS | 828 | -9.236 | -8.338 | -16.326 | 1.00 45.06 |
| ATOM | 5678 | CD | LYS | 828 | -8.689 | | -15.488 | 1.00 46.97 |
| ATOM | 5679 | CE | LYS | 828 | | -10.818 | | 1.00 47.07 |
| | 5680 | NZ | | 828 | | -11.962 | | 1.00 48.51 |
| ATOM | | | LYS | | | | | |
| ATOM | 5681 | C | LYS | 828 | -7.405 | | -15.737 | 1.00 32.78 |
| MOTA | 5682 | 0 | LYS | 828 | -7.356 | | -16.847 | 1.00 32.06 |
| ATOM | 5683 | N | PHE | 829 | -7.385 | | -14.608 | 1.00 29.83 |
| MOTA | 5684 | CA | PHE | 829 | -7.326 | -2.903 | -14.625 | 1.00 26.91 |
| MOTA | 5685 | CB | PHE | 829 | -7.961 | -2.332 | -13.350 | 1.00 25.84 |
| ATOM | 5686 | CG | PHE | 829 | -7.302 | -2.794 | -12.077 | 1.00 26.76 |
| ATOM | 5687 | CD1 | PHE | 829 | -6.061 | -2.289 | -11.684 | 1.00 25.54 |
| MOTA | 5688 | CD2 | PHE | 829 | -7.914 | -3.752 | -11.278 | 1.00 25.39 |
| ATOM | 5689 | CE1 | PHE | 829 | -5.447 | -2.739 | -10.514 | 1.00 27.51 |
| ATOM | 5690 | | PHE | 829 | -7.307 | | -10.112 | 1.00 27.40 |
| ATOM | 5691 | CZ | PHE | 829 | -6.071 | -3.697 | -9.728 | 1.00 26.75 |
| ATOM | 5692 | C | PHÉ | 829 | -5.923 | | -14.789 | 1.00 26.04 |
| | 5693 | | | 829 | -5.766 | | -15.010 | 1.00 26.02 |
| ATOM | | 0 | PHE | | | | | 1.00 24.63 |
| ATOM | 5694 | N | ALA | 830 | -4.910 | | -14.681 | |
| | 5695 | CA | ALA | 830 | -3.529 | | -14.813 | 1.00 23.28 |
| ATOM | 5696 | CB | ALA | 830 | -2.643 | | -13.828 | 1.00 21.79 |
| ATOM | 5697 | С | ALA | 830 | -2.997 | | -16.229 | 1.00 22.75 |
| MOTA | 5698 | 0 | ALA | 830 | -3.612 | -3.579 | -17.062 | 1.00 21.73 |
| ATOM | 5699 | N | LYS | 831 | -1.842 | -2.316 | -16.495 | 1.00 21.73 |
| ATOM | 5700 | CA | LYS | 831 | -1.209 | 2.421 | -17.801 | 1.00 20.75 |
| ATOM | 5701 | CB | LYS | 831 | -1.694 | -1.305 | -18.731 | 1.00 22.17 |
| MOTA | 5702 | CG | LYS | 831 | -0.965 | | -20.074 | 1.00 22.12 |
| MOTA | 5703 | CD | LYS | 831 | -1.486 | | -20.950 | 1.00 24.84 |
| ATOM | 5704 | CE | LYS | 831 | -0.669 | | -22.227 | 1.00 27.33 |
| ATOM | 5705 | NZ | LYS | 831 | -1.132 | | -23.117 | 1.00 27.97 |
| | | | | | 0.304 | | -17.665 | 1.00 27.37 |
| ATOM | 5706 | C. | LYS | 831 | | | -16.924 | |
| ATOM | 5707 | 0 | LYS | 831 | 0.839 | | | 1.00 20.39 |
| MOTA | 5708 | N | ASN | 832 | 0.985 | | -18.387 | 1.00 20.11 |
| MOTA | 5709 | CA | ASN | 832 | 2.442 | | -18.393 | 1.00 20.06 |
| MOTA | 5710 | CB | ASN | 832 | 2.915 | | -18.715 | 1.00 19.73 |
| MOTA | 5711 | CG | ASN | 832 | 4.430 | -4.820 | -18.755 | 1.00 19.21 |
| MOTA | 5712 | OD1 | ASN | 832 | 5.145 | -3.832 | -18.897 | 1.00 21.54 |
| ATOM | 5713 | ND2 | ASN | 832 | 4.921 | -6.045 | -18.653 | 1.00 18.62 |
| MOTA | 5714 | С | ASN | 832 | 2.933 | -2.323 | -19.480 | 1.00 20.14 |
| ATOM | 5715 | ō | ASN | 832 | 2.993 | | -20.653 | 1.00 19.00 |
| ATOM | 5716 | N | PHE | 833 | 3.283 | | -19.087 | 1.00 20.67 |
| ATOM | 5717 | CA | PHE | 833 | 3.764 | | -20.034 | 1.00 20.91 |
| | 5718 | CB | | · 833 | 3.696 | | -19.418 | 1.00 20.31 |
| MOTA | | | | | | | | 1.00 21.37 |
| MOTA | 5719 | CG CD1 | PHE | 833 | 2.298 | | -19.229 -18.075 | |
| ATOM | 5720 | CD1 | | 833 | 1.581 | | | 1.00 21.53 |
| MOTA | 5721 | CD2 | PHE | 833 | 1.679 | | -20.228 | 1.00 20.96 |
| MOTA | 5722 | CE1 | | 833 | 0.268 | | -17.919 | 1.00 23.22 |
| MOTA | 5723 | CE2 | PHE | 833 | 0.367 | | -20.081 | 1.00 22.83 |
| ATOM | 5724 | CZ | PHE | 833 | -0.345 | | -18.926 | 1.00 21.37 |
| MOTA | 5725 | С | PHE | 833 | 5.180 | -0.373 | -20.526 | 1.00 21.48 |
| ATOM | 5726 | 0 | PHE | 833 | 5.595 | 0.162 | -21.556 | 1.00 22.31 |

| ATOM | 5727 | N | LEU | 834 | 5.919 | -1.201 | -19.793 | 1.00 19.73 |
|------|-------|-----|-------------|-----|--------|--------|---------|-------------|
| ATOM | 5728 | CA | LEU | 834 | 7.289 | -1.541 | -20.176 | 1.00 20.43 |
| ATOM | 5729 | CB | LEU | 834 | 8.037 | -2.176 | -18.999 | 1.00 19.89 |
| ATOM | 5730 | CG | LEU | 834 | 9.493 | | -19.278 | 1.00 18.42 |
| ATOM | 5731 | CD1 | | 834 | 10.312 | | -19.481 | 1.00 21.54 |
| | 5732 | CD2 | LEU | 834 | 10.064 | | -18.115 | 1.00 20.29 |
| MOTA | | | | | | | -21.348 | 1.00 20.23 |
| ATOM | 5733 | C | LEU | 834 | 7.301 | | | |
| ATOM | 5734 | 0 | LEU | 834 | 8.221 | | -22.163 | 1.00 22.86 |
| ATOM | 5735 | N | ALA | 835 | 6.284 | | -21.419 | 1.00 25.29 |
| MOTA | 5736 | CA | ALA | 835 | 6.190 | -4.332 | -22.504 | 1.00 29.51 |
| ATOM | 5737 | CB | ALA | 835 | 4.968 | -5.221 | -22.310 | 1.00 30.38 |
| ATOM | 5738 | С | ALA | 835 | 6.086 | -3.582 | -23.824 | 1.00 32.18 |
| ATOM | 5739 | 0 | ALA | 835 | 6.775 | -3.911 | -24.789 | 1.00 32.05 |
| ATOM | 5740 | N | GLU | 836 | 5.207 | -2.581 | -23.843 | 1.00 34.79 |
| ATOM | 5741 | CA | GLU | 836 | 4.973 | | -25.013 | 1.00 38.46 |
| ATOM | 5742 | CB | GLU | 836 | 4.016 | | -24.664 | 1.00 41.47 |
| | | | | | | | -24.239 | 1.00 45.34 |
| MOTA | 5743 | CG | GLU | 836 | 2.611 | | | |
| MOTA | 5744 | CD | GLU | 836 | 1.726 | | -25.417 | 1.00 47.52 |
| MOTA | 5745 | OE1 | | 836 | 2.091 | | -26.160 | 1.00 48.57 |
| MOTA | 5746 | OE2 | GLU | 836 | 0.670 | | -25.598 | 1.00 48.67 |
| MOTA | 5747 | С | GLU | 836 | 6.304 | -1.151 | -25.450 | 1.00 38.72 |
| MOTA | 5748 | 0 | GLU | 836 | 6.690 | -1.249 | -26.612 | 1.00 41.32 |
| MOTA | 5749 | N | THR | 837 | 6.997 | -0.524 | -24.506 | 1.00 37.17 |
| ATOM | 5750 | CA | THR | 837 | 8.284 | 0.072 | -24.796 | 1.00 36.61 |
| ATOM | 5751 | CB | THR | 837 | 8.505 | | -23.987 | 1.00 36.83 |
| ATOM | 5752 | OG1 | THR | 837 | 9.822 | | -24.253 | 1.00 38.80 |
| ATOM | 5753 | CG2 | THR | 837 | 8.351 | | -22.489 | 1.00 35.24 |
| ATOM | 5754 | C | THR | 837 | 9.393 | | -24.480 | 1.00 36.87 |
| | | | | | | | | |
| ATOM | 5755 | 0 | THR | 837 | 9.207 | | -24.616 | 1.00 38.89 |
| MOTA | 5756 | N | GLY | 838 | 10.546 | | -24.067 | 1.00 33.88 |
| ATOM | 5757 | CA | GLY | 838 | 11.662 | | -23.738 | 1.00 31.57 |
| MOTA | 5758 | С | GLY | 838 | 12.514 | | -22.640 | 1.00 28.89 |
| MOTA | 5759 | 0 | GLY | 838 | 13.484 | | -22.201 | 1.00 28.70 |
| MOTA | 5760 | N | ASP | 839 | 12.126 | 0.511 | -22.186 | 1.00 28.03 |
| MOTA | 5761 | CA | ASP | 839 | 12.852 | 1.236 | -21.154 | 1.00 27.44 |
| ATOM | 5762 | CB | ASP | 839 | 13.574 | 2.410 | -21.834 | 1.00 32.86 |
| ATOM | 5763 | CG | ASP | 839 | 14.173 | 3.381 | -20.859 | 1.00 35.56 |
| MOTA | 5764 | OD1 | ASP | 839 | 13.475 | 4.350 | -20.483 | 1.00 36.98 |
| ATOM | 5765 | | ASP | 839 | 15.347 | | -20.470 | 1.00 40.04 |
| ATOM | 5766 | C | ASP | 839 | 11.886 | | -20.054 | 1.00 24.78 |
| ATOM | 5767 | o | ASP | 839 | 10.805 | | -20.349 | 1.00 24.31 |
| | 5768. | N | ILE | 840 | 12.274 | | -18.789 | 1.00 24.51 |
| MOTA | | | | | | | -17.671 | 1.00 22.00 |
| MOTA | 5769 | CA | ILE | 840 | 11.418 | | | |
| MOTA | 5770 | CB | ILE | 840 | 12.087 | | -16.306 | 1.00 17.83 |
| ATOM | 5771 | CG2 | ILE | 840 | 11.244 | | -15.154 | 1.00 17.98 |
| ATOM | 5772 | CG1 | ILE | 840 | 12.249 | | -16.168 | 1.00 18.15 |
| MOTA | 5773 | CD1 | $_{ m ILE}$ | 840 | 12.960 | | -14.889 | 1.00 21.02 |
| MOTA | 5774 | С | ILE | 840 | 11.034 | | -17.708 | 1.00 18.92 |
| MOTA | 5775 | 0 | ILE | 840 | 9.879 | 3.783 | -17.473 | 1.00 18.54 |
| MOTA | 5776 | N | ARG | 841 | 11.998 | 4.300 | -17.995 | 1.00 19.90 |
| ATOM | 5777 | CA | ARG | 841 | 11.698 | 5.722 | -18.067 | 1.00 .19.12 |
| ATOM | 5778 | CB | ARG | 841 | 12.991 | 6.530 | -18.204 | 1.00 18.56 |
| ATOM | 5779 | CG | ARG | 841 | 13.814 | | -16.916 | 1.00 20.62 |
| ATOM | 5780 | CD | ARG | 841 | 15.181 | | -17.067 | 1.00 21.49 |
| ATOM | 5781 | NE | ARG | 841 | 15.852 | | -15.774 | 1.00 21.43 |
| ATOM | 5782 | CZ | ARG | 841 | 16.347 | | -15.082 | 1.00 22.30 |
| ATOM | 5783 | | ARG | 841 | 16.260 | | -15.556 | 1.00 22.30 |
| | | | | | | | | |
| ATOM | 5784 | | ARG | 841 | 16.914 | | -13.902 | 1.00 22.06 |
| ATOM | 5785 | C | ARG | 841 | 10.743 | | -19.232 | 1.00 18.94 |
| ATOM | 5786 | 0 | ARG | 841 | 9.842 | | -19.132 | 1.00 17.46 |
| MOTA | 5787 | N | ALA | 842 | 10.918 | | -20.331 | 1.00 19.89 |
| MOTA | 5788 | CA | ALA | 842 | 10.028 | | -21.469 | 1.00 20.59 |
| ATOM | 5789 | CB | ALA | 842 | 10.558 | | -22.677 | 1.00 22.80 |
| ATOM | 5790 | С | ALA | 842 | 8.638 | 4.921 | -21.091 | 1.00 20.77 |
| ATOM | 5791 | 0 | ALA | 842 | 7.624 | 5.422 | -21.583 | 1.00 22.42 |
| ATOM | 5792 | N | ALA | 843 | 8.591 | | -20.214 | 1.00 19.81 |
| ATOM | 5793 | CA | ALA | 843 | 7.320 | | -19.780 | 1.00 17.80 |
| ATOM | 5794 | СВ | ALA | 843 | 7.566 | | -19.019 | 1.00 19.09 |
| ATOM | 5795 | C | ALA | 843 | 6.539 | | -18.910 | 1.00 17.75 |
| ATOM | 5796 | 0 | ALA | 843 | 5.310 | | -19.002 | 1.00 17.73 |
| | 5797 | | | 844 | 7.259 | | -18.059 | 1.00 13.71 |
| MOTA | | N | VAL | | | | -17.183 | 1.00 17.72 |
| ATOM | 5798 | CA | VAL | 844 | 6.647 | | | |
| ATOM | 5799 | CB | VAL | 844 | 7.683 | | -16.185 | 1.00 15.55 |
| ATOM | 5800 | | VAL | 844 | 7.074 | | -15.448 | 1.00 18.17 |
| ATOM | 5801 | | VAL | 844 | 8.113 | | -15.169 | 1.00 15.06 |
| ATOM | 5802 | С | VAL | 844 | 6.063 | | -18.029 | 1.00 19.69 |
| ATOM | 5803 | 0 | VAL | 844 | 4.942 | 7.606 | -17.790 | 1.00 19.85 |
| | | | | | | | | |

| ATOM | 5804 | N | ARG | 845 | 6.817 | 7.618 -19.024 | 1.00 20.79 |
|------|------|-----|-----|------|--------|----------------|------------|
| ATOM | 5805 | CA | ARG | 845 | 6.325 | 8.695 -19.876 | 1.00 21.40 |
| | | | | | | | |
| MOTA | 5806 | CB | ARG | 845 | 7.394 | 9.118 -20.886 | 1.00 23.26 |
| MOTA | 5807 | CG | ARG | 845 | 8.621 | 9.752 -20.255 | 1.00 24.31 |
| MOTA | 5808 | CD | ARG | 845 | 9.502 | 10.422 -21.298 | 1.00 25.50 |
| ATOM | 5809 | NE | ARG | 845 | 10.126 | 9.470 -22.217 | 1.00 25.46 |
| ATOM | 5810 | CZ | ARG | 845 | 11.294 | 8.872 -22.001 | 1.00 26.44 |
| | | | | 845 | 11.976 | 9.121 -20.890 | 1.00 27.41 |
| MOTA | 5811 | | ARG | | | | |
| MOTA | 5812 | | ARG | 845 | 11.787 | 8.038 -22.908 | 1.00 24.69 |
| ATOM | 5813 | С | ARG | 845 | 5.054 | 8.281 -20.612 | 1.00 21.24 |
| MOTA | 5814 | 0 | ARG | 845 | 4.109 | 9.068 -20.733 | 1.00 19.90 |
| ATOM | 5815 | N | GLN | 846 | 5.029 | 7.044 -21.100 | 1.00 20.09 |
| ATOM | 5816 | CA | GLN | 846 | 3.862 | 6.549 -21.816 | 1.00 20.80 |
| ATOM | 5817 | СВ | GLN | 846 | 4.140 | 5.163 -22.410 | 1.00 23.28 |
| | | | | 846 | | | |
| MOTA | 5818 | CG | GLN | | 2.932 | 4.529 -23.092 | |
| MOTA | 5819 | CD | GLN | 846 | 3.280 | 3.266 -23.869 | 1.00 35.73 |
| MOTA | 5820 | OE1 | GLN | 846 | 3.947 | 3.324 -24.904 | 1.00 38.70 |
| MOTA | 5821 | NE2 | GLN | 846 | 2.833 | 2.117 -23.370 | 1.00 37.15 |
| ATOM | 5822 | С | GLN | 846 | 2.652 | 6.498 -20.889 | 1.00 19.10 |
| ATOM | 5823 | 0 | GLN | 846 | 1.527 | 6.809 -21.290 | 1.00 18.61 |
| ATOM | 5824 | N | TYR | 847 | 2.881 | 6.117 -19.639 | 1.00 18.58 |
| | | | | | | | |
| MOTA | 5825 | CA | TYR | 847 | 1.790 | 6.051 -18.676 | 1.00 18.17 |
| MOTA | 5826 | CB | TYR | 847 | 2.301 | 5.446 -17.365 | 1.00 17.16 |
| MOTA | 5827 | CG | TYR | 847 | 1.364 | 5.597 -16.189 | 1.00 14.88 |
| MOTA | 5828 | CD1 | TYR | 847. | 0.037 | 5.160 -16.257 | 1.00 13.94 |
| MOTA | 5829 | CE1 | TYR | 847 | -0.810 | 5.277 -15.156 | 1.00 14.43 |
| MOTA | 5830 | | TYR | 847 | 1.814 | 6.152 -14.995 | 1.00 14.30 |
| ATOM | 5831 | | TYR | 847 | 0.980 | 6.272 -13.897 | 1.00 13.19 |
| | | | TYR | | -0.321 | 5.839 -13.975 | 1.00 14.15 |
| ATOM | 5832 | CZ | | 847 | | | |
| MOTA | 5833 | ОН | TYR | 847 | -1.130 | 5.965 -12.876 | 1.00 15.40 |
| MOTA | 5834 | С | TYR | 847 | 1.222 | 7.453 -18.451 | 1.00 17.79 |
| MOTA | 5835 | 0 | TYR | 847 | 0.005 | 7.646 -18.429 | 1.00 18.16 |
| ATOM | 5836 | N | MET | 848 | 2.112 | 8.430 -18.299 | 1.00 19.31 |
| ATOM | 5837 | CA | MET | 848 | 1.705 | 9.813 -18.089 | 1.00 19.23 |
| | 5838 | CB | MET | 848 | 2.946 | 10.700 -17.931 | 1.00 21.20 |
| MOTA | 5839 | CG | MET | 848 | 3.724 | 10.462 -16.639 | 1.00 21.47 |
| | | | | | | | |
| MOTA | 5840 | SD | MET | 848 | 5.424 | 11.088 -16.716 | 1.00 22.85 |
| ATOM | 5841 | CE | MET | 848 | 5.109 | 12.850 -16.646 | 1.00 23.08 |
| ATOM | 5842 | С. | MET | 848 | 0.861 | 10.304 -19.263 | 1.00 19.69 |
| MOTA | 5843 | 0 | MET | 848 | -0.208 | 10.882 -19.075 | 1.00 19.25 |
| ATOM | 5844 | N | ALA | 849 | 1.339 | 10.051 -20.476 | 1.00 20.45 |
| MOTA | 5845 | CA | ALA | 849 | 0.643 | 10.487 -21.681 | 1.00 20.76 |
| ATOM | 5846 | СВ | ALA | 849 | 1.537 | 10.280 -22.894 | 1.00 20.70 |
| | | | | 849 | -0.701 | 9.797 -21.892 | 1.00 20.70 |
| ATOM | 5847 | С | ALA | | | | |
| MOTA | 5848 | 0 | ALA | 849 | -1.699 | 10.456 -22.169 | 1.00 22.23 |
| MOTA | 5849 | N | GLU | 850 | -0.740 | 8.475 -21.761 | 1.00 19.51 |
| MOTA | 5850 | CA | GLU | 850 | -1.996 | 7.759 -21.960 | 1.00 20.22 |
| ATOM | 5851 | CB | GLU | 850 | -1.751 | 6.250 -21.977 | 1.00 20.03 |
| ATOM | 5852 | CG | GLU | 850 | -1.091 | 5.780 -23.261 | 1.00 21.40 |
| ATOM | 5853 | CD | GLU | 850 | -0.997 | 4.282 -23.355 | 1.00 22.09 |
| ATOM | 5854 | | GLU | 850 | -1.802 | 3.593 -22.703 | 1.00 23.56 |
| | | | | | | | |
| MOTA | 5855 | | GLU | 850 | -0.124 | 3.792 -24.096 | 1.00 27.29 |
| MOTA | 5856 | С | GLU | 850 | -3.075 | 8.108 -20.942 | 1.00 20.17 |
| MOTA | 5857 | 0 | GLU | 850 | -4.268 | 7.947 -21.211 | 1.00 20.44 |
| MOTA | 5858 | N | VAL | 851 | -2.666 | 8.574 -19.765 | 1.00 20.20 |
| ATOM | 5859 | CA | VAL | 851 | -3.642 | 8.967 -18.752 | 1.00 18.55 |
| MOTA | 5860 | CB | VAL | 851 | -2.995 | 9.092 -17.352 | 1.00 19.02 |
| MOTA | 5861 | | VAL | 851 | -3.957 | 9.783 -16.387 | 1.00 13.86 |
| ATOM | 5862 | | VAL | 851 | -2.663 | 7.700 -16.820 | 1.00 17.16 |
| | 5863 | | VAL | 851 | -4.266 | 10.305 -19.154 | 1.00 18.95 |
| ATOM | | С | | | | | 1.00 18.93 |
| ATOM | 5864 | 0 | VAL | 851 | -5.489 | | |
| ATOM | 5865 | N | GLU | 852 | -3.424 | 11.270 -19.506 | 1.00 20.35 |
| MOTA | 5866 | CA | GLU | 852 | -3.918 | 12.583 -19.895 | 1.00 22.19 |
| ATOM | 5867 | CB | GLU | 852 | -2.748 | 13.567 -20.023 | 1.00 24.34 |
| MOTA | 5868 | CG | GLU | 852 | -3.173 | 14.986 -20.385 | 1.00 28.53 |
| ATOM | 5869 | CD | GLU | 852 | -2.073 | 16.009 -20.170 | 1.00 30.90 |
| ATOM | 5870 | | GLU | 852 | -2.210 | 17.137 -20.687 | 1.00 35.44 |
| | | | | | -1.079 | 15.696 -19.480 | 1.00 33.44 |
| ATOM | | OE2 | GLU | 852 | | | |
| MOTA | 5872 | C | GLU | 852 | -4.745 | 12.560 -21.186 | 1.00 22.60 |
| MOTA | 5873 | 0 | GLU | 852 | -5.634 | 13.393 -21.376 | 1.00 21.58 |
| MOTA | 5874 | N | SER | 853 | -4.465 | 11.602 -22.064 | 1.00 23.29 |
| ATOM | 5875 | CA | SER | 853 | -5.204 | 11.489 -23.322 | 1.00 24.06 |
| MOTA | 5876 | CB | SER | 853 | -4.340 | 10.844 -24.405 | 1.00 26.77 |
| MOTA | 5877 | OG | SER | 853 | -3.358 | 11.747 -24.879 | 1.00 34.21 |
| ATOM | 5878 | C | SER | 853 | -6.473 | 10.671 -23.162 | 1.00 23.46 |
| ATOM | | | | | -7.340 | 10.690 -24.033 | 1.00 21.96 |
| | 5879 | 0 | SER | 853 | | | |
| ATOM | 5880 | N | GLY | 854 | -6.576 | 9.948 -22.052 | 1.00 20.67 |
| | | | | | | | |

| ATOM | 5881 | CA | GLY | 854 | -7.752 | 9.131 | -21.822 | 1.00 21.47 |
|------|------|-------------|-----|-----|---------|--------------------|----------------------|------------|
| ATOM | 5882 | С | GLY | 854 | -7.620 | 7 744 | -22.424 | 1.00 21.43 |
| | | | | | | | | |
| ATOM | 5883 | 0 | GLY | 854 | -8.552 | | -22.343 | 1.00 22.20 |
| MOTA | 5884 | N | VAL | 855 | -6.472 | 7.459 | -23.032 | 1.00 21.89 |
| ATOM | 5885 | CA | VAL | 855 | -6.210 | 6.151 | -23.636 | 1.00 22.78 |
| ATOM | 5886 | CB | VAL | 855 | -4.871 | 6.155 | -24.394 | 1.00 23.64 |
| | | | | | | | | |
| MOTA | 5887 | | VAL | 855 | -4.521 | | -24.855 | 1.00 25.02 |
| ATOM | 5888 | CG2 | VAL | 855 | -4.967 | 7.087 | -25.588 | 1.00 27.01 |
| ATOM | 5889 | С | VAL | 855 | -6.160 | 5.071 | -22.562 | 1.00 22.02 |
| | 5890 | ō | VAL | 855 | -6.572 | | -22.787 | 1.00 21.37 |
| ATOM | | | | | | | | |
| MOTA | 5891 | N | TYR | 856 | -5.632 | | -21.400 | 1.00 20.96 |
| ATOM | 5892 | CA | TYR | 856 | -5.530 | 4.551 | -20.252 | 1.00 19.68 |
| ATOM | 5893 | CB | TYR | 856 | -4.073 | 4.276 | -19.887 | 1.00 17.64 |
| ATOM | 5894 | CG | TYR | 856 | -3.966 | ं 3 3 1 9 . | -18.729 | 1.00 18.23 |
| | | | | | | | | |
| MOTA | 5895 | CD1 | TYR | 856 | -4.153 | | -18.923 | 1.00 17.91 |
| MOTA | 5896 | CE1 | TYR | 856 | -4.151 | 1.068 | -17.849 | 1.00 17.59 |
| ATOM | 5897 | CD2 | TYR | 856 | -3.766 | 3.782 | -17.424 | 1.00 19.26 |
| ATOM | 5898 | CE2 | TYR | 856 | -3.763 | | -16.339 | 1.00 16.18 |
| | | | | | | | | |
| MOTA | 5899 | cz | TYR | 856 | -3.958 | | -16.560 | 1.00 18.50 |
| MOTA | 5900 | OH | TYR | 856 | -3.975 | 0.676 | -15.494 | 1.00 19.57 |
| ATOM | 5901 | С | TYR | 856 | -6.208 | 5.195 | -19.048 | 1.00 19.48 |
| ATOM | 5902 | 0 | TYR | 856 | -5.951 | | -18.735 | 1.00 18.59 |
| | | | | | | | | |
| MOTA | 5903 | N | PRO | 857 | -7.057 | | -18.339 | 1.00 21.09 |
| MOTA | 5904 | $^{\rm CD}$ | PRO | 857 | -7.690 | 4.858 | -17.079 | 1.00 22.39 |
| MOTA | 5905 | CA | PRO | 857 | -7.373 | 3.034 | -18.631 | 1.00 22.76 |
| MOTA | 5906 | CB | PRO | 857 | -7.935 | 2 528 | -17.309 | 1.00 23.94 |
| | | | | | | | | |
| MOTA | 5907 | CG | PRO | 857 | -8.658 | | -16.794 | 1.00 24.29 |
| MOTA | 5908 | С | PRO | 857 | -8.355 | 2.860 | -19.784 | 1.00 23.68 |
| MOTA | 5909 | 0 | PRO | 857 | -9.263 | 3.670 | -19.970 | 1.00 22.22 |
| ATOM | 5910 | N · | | 858 | -8.166 | | -20.558 | 1.00 24.27 |
| | | | | | | | -21.684 | 1.00 24.39 |
| MOTA | 5911 | CA | GLY | 858 | -9.048 | | | |
| MOTA | 5912 | С | GLY | 858 | -10.250 | 0.719 | -21.272 | 1.00 25.24 |
| MOTA | 5913 | 0 | GLY | 858 | -10.357 | 0.297 | -20,122 | 1.00 23.87 |
| ATOM | 5914 | N | GLU | 859 | -11.165 | | -22.205 | 1.00 25.45 |
| | | | | | | | | 1.00 28.69 |
| MOTA | 5915 | CA | GLU | 859 | -12.344 | | -21.891 | |
| MOTA | 5916 | CB | GLU | 859 | -13.185 | -0.520 · | -23.151 _. | 1.00 31.54 |
| MOTA | 5917 | CG | GLU | 859 | -14.435 | -1.339 | -22.908 | 1.00 34.32 |
| MOTA | 5918 | CD | GLU | 859 | -15.420 | -0.640 | -21.992 | 1.00 37.49 |
| | | | | | -16.335 | -1.318 | | 1.00 40.17 |
| MOTA | 5919 | | GLU | 859 | | | | |
| ATOM | 5920 | OE2 | GLU | 859 | -15.284 | | -21.787 | 1.00 37.73 |
| MOTA | 5921 | C | GLU | 859 | -11.911 | -1.650 | -21.312 | 1.00 28.31 |
| ATOM | 5922 | 0 | GLU | 859 | -12.585 | -2.207 | -20.446 | 1.00 28.91 |
| | 5923 | N | GLU | 860 | -10.774 | | -21.779 | 1.00 30.25 |
| MOTA | | | | | | | | |
| MOTA | 5924 | CA | GLU | 860 | -10.255 | -3.448 | | 1.00 31.44 |
| MOTA | 5925 | CB | GLU | 860 | -9.016 | -3.851 | -22.119 | 1.00 35.44 |
| MOTA | 5926 | CG | GLU | 860 | -9.077 | -3.503 | -23.593 | 1.00 41.38 |
| ATOM | 5927 | CD | GLU | 860 | -8.747 | -2.044 | | 1.00 43.62 |
| | | | | | | | | |
| MOTA | 5928 | | GLU | 860 | -7.599 | -1.637 | | 1.00 44.99 |
| ATOM | 5929 | OE2 | GLU | 860 | -9.633 | -1.306 | -24.342 | 1.00 44.03 |
| ATOM | 5930 | С | GLU | 860 | -9.887 | -3.455 | -19.833 | 1.00 31.02 |
| ATOM | 5931 | 0 | GLU | 860 | -9.957 | -4.494 | | 1.00 30.50 |
| | | | | | | -2.296 | | 1.00 28.81 |
| ATOM | 5932 | N | HIS | 861 | -9.488 | | | |
| MOTA | 5933 | CA | HIS | 861 | -9.087 | | -17.915 | 1.00 27.99 |
| ATOM | 5934 | CB | HIS | 861 | -7.934 | $-1.170 \cdot$ | -17.793 | 1.00 25.91 |
| MOTA | 5935 | CG | HIS | 861 | -6.871 | -1.344 | -18.828 | 1.00 24.41 |
| ATOM | 5936 | | HIS | 861 | -6.519 | -0.568 | | 1.00 22.82 |
| | | | | | | | | |
| MOTA | 5937 | - | HIS | 861 | -6.026 | -2.432 | | 1.00 25.29 |
| MOTA | 5938 | CE1 | HIS | 861 | -5.199 | -2.319 | | 1.00 22.41 |
| ATOM | 5939 | NE2 | HIS | 861 | -5.478 | -1.197 | -20.518 | 1.00 24.27 |
| ATOM | 5940 | С | HIS | 861 | -10.235 | -1.677 | | 1.00 27.60 |
| | | | | | -10.042 | -1.385 | | |
| MOTA | 5941 | 0 | HIS | 861 | | | | 1.00 27.53 |
| MOTA | 5942 | N | SER | 862 | -11.427 | -1.594 - | | 1.00 26.94 |
| ATOM | 5943 | CA | SER | 862 | -12.580 | -1.096 · | -16.888 | 1.00 27.95 |
| ATOM | 5944 | CB | SER | 862 | -13.240 | | -17.686 | 1.00 27.74 |
| | | OG | | 862 | -12.273 | | -18.118 | 1.00 28.11 |
| MOTA | 5945 | | SER | | | | | |
| MOTA | 5946 | С | SER | 862 | -13.620 | -2.160 · | | 1.00 29.39 |
| MOTA | 5947 | 0 | SER | 862 | -13.764 | -3.156 | -17.258 | 1.00 28.79 |
| MOTA | 5948 | N | PHE | 863 | -14.336 | -1.936 | -15.447 | 1.00 29.95 |
| ATOM | 5949 | CA | PHE | 863 | -15.385 | -2.842 | | 1.00 32.29 |
| | | | | | | | | |
| MOTA | 5950 | CB | PHE | 863 | -15.257 | -3.141 | | 1.00 30.67 |
| ATOM | 5951 | CG | PHE | 863 | -13.991 | -3.858 | | 1.00 31.07 |
| ATOM | 5952 | CD1 | PHE | 863 | -12.912 | -3.160 - | -12.587 | 1.00 31.09 |
| ATOM | 5953 | | PHE | 863 | -13.875 | -5.234 | | 1.00 31.78 |
| | | | | | | -3.820 - | | 1.00 30.30 |
| MOTA | 5954 | | PHE | 863 | -11.737 | | | |
| ATOM | 5955 | CE2 | PHE | 863 | -12.703 | -5.905 | | 1.00 32.24 |
| ATOM | 5956 | CZ | PHE | 863 | -11.633 | -5.195 | -12.413 | 1.00 32.64 |
| ATOM | 5957 | С | PHE | 863 | -16.741 | -2.197 | -15.261 | 1.00 34.00 |
| | | - | | | | - | | |

| ATOM | 5958 | 0 | PHE | 863 | -16.8 | 319 | -1.031 | -15.651 | 1.00 | 34.45 |
|------|------|------|----------------|-----|-------|-----|---------|---------|------|-------|
| ATOM | 5959 | N | HIS | 864 | -17.8 | | | -15.042 | 1.00 | 35.05 |
| ATOM | 5960 | CA | HIS | 864 | -19.1 | | | -15.252 | | 36.87 |
| | 5961 | CB | HIS | 864 | -19.6 | | | -16.700 | | 37.63 |
| ATOM | | | | | | | | -17.682 | | 37.41 |
| MOTA | 5962 | CG | HIS | 864 | -18.9 | | | | | |
| ATOM | 5963 | | HIS | 864 | -18.0 | | | -18.688 | | 38.33 |
| MOTA | 5964 | ND1 | HIS | 864 | -19.1 | 130 | -0.425 | -17.678 | 1.00 | 38.08 |
| ATOM | 5965 | CE1 | HIS | 864 | -18.4 | 108 | 0.123 | -18.639 | 1.00 | 37.64 |
| MOTA | 5966 | NE2 | HIS | 864 | -17.7 | 752 | -0.835 | -19.266 | 1.00 | 37.77 |
| ATOM | 5967 | С | HIS | 864 | -20.1 | | | -14.305 | 1.00 | 37.62 |
| MOTA | 5968 | Õ | HIS | 864 | -21.2 | | | -14.068 | | 38.24 |
| | | | | | -19.7 | | | | | 39.23 |
| MOTA | 5969 | | HIS | 864 | | | | -13.826 | | |
| MOTA | 5970 | C1 | KPL | 865 | -3.3 | | 0.634 | -5.095 | | 39.96 |
| MOTA | 5971 | C2 | \mathtt{KPL} | 865 | -3.5 | 550 | 1.896 | -4.226 | | 38.72 |
| ATOM | 5972 | C3 | KPL | 865 | -2.6 | 517 | 2.997 | -4.740 | 1.00 | 39.62 |
| ATOM | 5973 | C4 | KPL | 865 | -5.0 | 003 | 2.393 | -4.350 | 1.00 | 40.42 |
| ATOM | 5974 | 01 | KPL | 865 | -5.9 | 910 | 1.387 | -3.884 | 1.00 | 45.23 |
| ATOM | 5975 | C5 | KPL | 865 | -3.2 | | 1.589 | -2.749 | | 35.98 |
| ATOM | 5976 | 02 | KPL | 865 | -4.0 | | 1.753 | -1.886 | | 36.91 |
| | | | | | | | | | | |
| ATOM | 5977 | C6 | KPL | 865 | -1.8 | | 1.081 | -2.331 | | 32.68 |
| MOTA | 5978 | 03 | KPL | 865 | -0.9 | | 0.900 | -3.150 | | 30.34 |
| ATOM | 5979 | 04 | \mathtt{KPL} | 865 | -1.6 | | 0.826 | -1.028 | 1.00 | 27.08 |
| ATOM | 5980 | CB | MET | 901 | -12.7 | 712 | -23.902 | -0.148 | 1.00 | 60.92 |
| ATOM | 5981 | CG | MET | 901 | -12.5 | 590 | -25.152 | -1.024 | 1.00 | 62.73 |
| ATOM | 5982 | SD | MET | 901 | -10.8 | 391 | -25.631 | -1.435 | 1.00 | 65.23 |
| АТОМ | 5983 | CE | MET | 901 | | | -25.064 | -3.145 | | 64.55 |
| | 5984 | | MET | 901 | -10.8 | | -22.440 | -0.981 | | 58.43 |
| ATOM | | C | | | | | | | | |
| ATOM | 5985 | 0 | MET | 901 | -10.0 | | -23.083 | -0.258 | | 58.56 |
| MOTA | 5986 | N | MET | 901 | -13.0 | | -22.466 | -2.137 | | 59.24 |
| MOTA | 5987 | CA | MET | 901 | -12.3 | | -22.573 | -0.834 | | 59.60 |
| MOTA | 5988 | N | LYS | 902 | -10.4 | 115 | -21.594 | -1.912 | 1.00 | 56.21 |
| MOTA | 5989 | CA | LYS | 902 | -8.9 | 991 | -21.379 | -2.147 | 1.00 | 52.69 |
| ATOM | 5990 | СВ | LYS | 902 | | | -22.296 | -3.281 | | 54.41 |
| ATOM | 5991 | CG | LYS | 902 | -6.9 | | -22.462 | -3.364 | | 55.97 |
| | | | | | -6.3 | | -21.347 | -4.158 | | 57.24 |
| ATOM | 5992 | CD | LYS | 902 | | | | | | |
| MOTA | 5993 | CE | LYS | 902 | -6.6 | | -21.451 | -5.641 | | 58.67 |
| MOTA | 5994 | NZ | LYS | 902 | -5.9 | | -20.416 | -6.455 | | 59.28 |
| MOTA | 5995 | С | LYS | 902 | -8.7 | 721 | -19.915 | -2.491 | 1.00 | 49.10 |
| ATOM | 5996 | 0 | LYS | 902 | -8.6 | 88 | -19.538 | -3.664 | 1.00 | 49.44 |
| MOTA | 5997 | N | PRO | 903 | -8.5 | 542 | -19.065 | -1.465 | 1.00 | 44.68 |
| ATOM | 5998 | CD | PRO | 903 | -8.0 | 96 | -17.671 | -1.635 | 1.00 | 43.26 |
| ATOM | 5999 | CA | PRO | 903 | -8.5 | | -19.422 | -0.042 | | 40.59 |
| | | | | 903 | -7.8 | | -18.281 | 0.615 | | 41.44 |
| MOTA | 6000 | CB | PRO | | | | | | | |
| ATOM | 6001 | CG | PRO | 903 | -8.2 | | -17.114 | -0.230 | | 42.64 |
| ATOM | 6002 | С | PRO | 903 | | | -19.540 | 0.488 | | 37.14 |
| MOTA | 6003 | 0 | PRO | 903 | -10.9 | 957 | -19.042 | -0.125 | 1.00 | 35.87 |
| ATOM | 6004 | N | THR | 904 | -10.1 | L75 | -20.205 | 1.628 | 1.00 | 32.92 |
| MOTA | 6005 | CA | THR | 904 | -11.4 | 194 | -20.369 | 2.227 | 1.00 | 29.48 |
| ATOM | 6006 | CB - | THR | 904 | -11.5 | 504 | -21.543 | 3.238 | 1.00 | 29.39 |
| ATOM | 6007 | OG1 | | 904 | | | -22.764 | 2.565 | 1.00 | 26.97 |
| ATOM | 6008 | CG2 | | 904 | -12.8 | | -21.690 | 3.869 | 1.00 | |
| | | | | | | | -19.073 | 2.950 | | 28.40 |
| ATOM | 6009 | C | THR | 904 | | | | | | |
| ATOM | 6010 | 0 | THR | 904 | | | -18.560 | 3.739 | | 27.37 |
| ATOM | 6011 | N | THR | 905 | | | -18.543 | 2.675 | 1.00 | |
| ATOM | 6012 | CA | THR | 905 | | | -17.300 | 3.308 | 1.00 | 28.38 |
| ATOM | 6013 | CB | THR | 905 | -13.4 | 170 | -16.122 | 2.310 | 1.00 | 29.55 |
| MOTA | 6014 | OG1 | THR | 905 | -14.3 | 342 | -16.416 | 1.211 | 1.00 | 31.91 |
| ATOM | 6015 | CG2 | THR | 905 | -12.0 | 066 | -15.873 | 1.796 | 1.00 | 31.52 |
| ATOM | 6016 | С | THR | 905 | -14.8 | | -17.398 | 3.888 | 1.00 | 27.90 |
| ATOM | 6017 | ō | THR | 905 | -15.6 | | -18.380 | 3.670 | | 26.37 |
| | | | | | | | -16.370 | 4.633 | | 28.35 |
| MOTA | 6018 | N | ILE | 906 | -15.2 | | | | | |
| ATOM | 6019 | CA | | 906 | | | -16.331 | 5.244 | | 29.75 |
| ATOM | 6020 | CB | ILE | 906 | -16.8 | | -14.979 | 5.961 | | 30.43 |
| ATOM | 6021 | CG2 | | 906 | -18.1 | | -15.061 | 6.819 | | 29.82 |
| MOTA | 6022 | CG1 | ILE | 906 | -15.6 | | -14.641 | 6.856 | | 32.57 |
| MOTA | 6023 | CD1 | ILE | 906 | -15.6 | 538 | -13.192 | 7.341 | 1.00 | 34.53 |
| ATOM | 6024 | С | ILE | 906 | | | -16.505 | 4.151 | 1.00 | 30.16 |
| ATOM | 6025 | ō | ILE | 906 | -18.7 | | -17.073 | 4.384 | | 29.90 |
| ATOM | 6026 | N | SER | 907 | | | -16.021 | 2.955 | | 31.30 |
| | | | | | | | -16.107 | 1.810 | | 32.70 |
| MOTA | 6027 | CA | SER | 907 | | | | | | |
| MOTA | 6028 | CB | SER | 907 | | | -15.593 | 0.547 | | 33.26 |
| MOTA | 6029 | OG | SER | 907 | | | -14.332 | 0.770 | | 34.50 |
| MOTA | 6030 | C | SER | 907 | | | -17.544 | 1.581 | | 32.03 |
| MOTA | 6031 | 0 | SER | 907 | | | -17.793 | 1.255 | | 31.78 |
| ATOM | 6032 | N | LEU | 908 | -17.7 | 777 | -18.485 | 1.757 | 1.00 | 32.10 |
| ATOM | 6033 | CA | LEU | 908 | | | -19.900 | 1.563 | 1.00 | 31.83 |
| MOTA | 6034 | СВ | LEU | 908 | | | -20.723 | 1.643 | 1.00 | 33.59 |
| | | | | | | | | | | |

| N/IIOM | 6035 | CG | LEU | 908 | -16.563 | 21 705 | 0.566 | 1 00 | 35.17 |
|--|--|--|---|---|--|--|---|--|---|
| ATOM | | | | | | | | | 34.73 |
| MOTA | 6036 | | LEU | 908 | -15.600 | | 1.103 | | |
| MOTA | 6037 | CD2 | LEU | 908 | | -22.441 | 0.173 | | 36.87 |
| MOTA | 6038 | С | LEU | 908 | -19.073 | -20.437 | 2.586 | | 30.86 |
| ATOM | 6039 | .0 | LEU | 908 | -20.056 | -21.087 | 2.223 | 1.00 | 31.03 |
| ATOM | 6040 | N | LEU | 909 | -18.818 | -20.176 | 3.865 | 1.00 | 29.63 |
| ATOM | 6041 | CA | LEU | 909 | | -20.643 | 4.926 | | 28.90 |
| | 6042 | CB | LEU | 909 | -19.179 | | 6.297 | | 26.59 |
| MOTA | | | | | | | | | |
| MOTA | 6043 | CG | LEU | 909 | -17.783 | -20.723 | 6.669 | | 26.10 |
| MOTA | 6044 | | LEU | 909 | -17.476 | -20.315 | 8.102 | | 25.81 |
| ATOM | 6045 | CD2 | LEU | 909 | -17.721 | -22.229 | 6.519 | 1.00 | 27.17 |
| ATOM | 6046 | С | LEU | 909 | -21.109 | -20.093 | 4.750 | 1.00 | 29.37 |
| ATOM | 6047 | ō | LEU | 909 | -22.092 | | 5.056 | | 28.78 |
| | 6048 | N | GLN | 910 | | -18.861 | 4.266 | | 30.45 |
| ATOM | | | | | | | | | |
| MOTA | 6049 | CA | GLN | 910 | | -18.234 | 4.050 | | 33.43 |
| MOTA | 6050 | CB | GLN | 910 | -22.306 | | 3.659 | | 33.71 |
| MOTA | 6051 | CG | GLN | 910 | -23.589 | -15.949 | 3.626 | 1.00 | 37.45 |
| MOTA | 6052 | CD | GLN | 910 | -24.345 | -15.976 | 4.944 | 1.00 | 37.83 |
| ATOM | 6053 | | GLN | 910 | | -16.935 | 5.250 | 1.00 | 38.97 |
| ATOM | 6054 | NE2 | GLN | 910 | | -14.924 | | | 36.67 |
| | | | | | | | | | |
| MOTA | 6055 | С | GLN | 910 | -23.205 | -19.006 | 2.945 | | 33.53 |
| MOTA | 6056 | 0 | GLN | 910 | | -19.258 | 3.028 | | 33.64 |
| MOTA | 6057 | N | LYS | 911 | -22.451 | -19.389 | 1.919 | 1.00 | 35.95 |
| ATOM | 6058 | CA | LYS | 911 | -23.004 | -20.154 | 0.811 | 1.00 | 36.69 |
| MOTA | 6059 | СВ | LYS | 911 | -21.947 | -20.387 | -0.269 | 1.00 | 38.54 |
| ATOM | 6060 | CG | LYS | 911 | -22.480 | -21.146 | -1.478 | | 41.44 |
| | | | | | | | | | |
| MOTA | 6061 | CD | LYS | 911 | | -22.170 | -2.010 | | 42.22 |
| MOTA | 6062 | CE | LYS | 911 | | -21.525 | -2.522 | | 43.30 |
| MOTA | 6063 | NZ | LYS | 911 | -19.319 | -22.540 | -3.158 | 1.00 | 44.28 |
| MOTA | 6064 | С | LYS | 911 | -23.488 | -21.504 | 1.326 | 1.00 | 36.17 |
| MOTA | 6065 | 0 | LYS | 911 | -24.545 | -21.989 | 0.927 | 1.00 | 36.29 |
| ATOM | | · N | TYR | 912 | | -22.108 | 2.214 | | 35.44 |
| | | | | | -23.041 | | 2.789 | | 33.78 |
| ATOM | 6067 | CA ⁻ | TYR | 912 | | | | | |
| MOTA | 6068 | CB | TYR | 912 | -21.945 | -23.862 | 3.758 | | 35.49 |
| MOTA | 6069 | CG | TYR | 912 | -20.707 | -24.422 | 3.091 | | 37.41 |
| ATOM | 6070 | CD1 | TYR | 912 | -19.533 | -24.628 | 3.820 | 1.00 | 38.67 |
| ATOM | 6071 | CE1 | TYR | 912 | -18.395 | -25.159 | 3.217 | 1.00 | 39.92 |
| MOTA | 6072 | CD2 | TYR | 912 | -20.710 | -24.766 | 1.737 | | 38.60 |
| ATOM | 6073 | CE2 | TYR | 912 | -19.580 | -25.299 | 1.127 | | 40.16 |
| | | | | | | | | | |
| MOTA | 6074 | CZ | TYR | 912 | -18.428 | -25.493 | 1.871 | | 40.30 |
| MOTA | 6075 | OH | TYR | 912 | -17.310 | -26.021 | 1.270 | | 42.12 |
| MOTA | 6076 | C | TYR | 912 | -24.375 | -23.390 | 3.516 | 1.00 | 33.39 |
| MOTA | 6077 | 0 | TYR | 912 | -25.128 | -24.359 | 3.460 | 1.00 | 31.55 |
| MOTA | 6078 | N | LYS | 913 | -24.663 | -22.297 | 4.211 | 1.00 | 32.88 |
| MOTA | 6079 | CA | LYS | 913 | -25.920 | -22.202 | 4.936 | | 35.58 |
| | | | | | | | 5.878 | | 33.03 |
| MOTA | 6080 | CB | LYS | 913 | | -20.999 | | | |
| ATOM | 6081 | CG | LYS | 913 . | | -20.898 | 6.697 | | 32.07 |
| MOTA | 6082 | CD | LYS | 913 | -27.072 | -19.884 | 7.815 | 1.00 | 29.62 |
| MOTA | 6083 | CE | LYS | 913 | -28.360 | -19.861 | 8.616 | 1.00 | 28.34 |
| ATOM | 6084 | NZ | LYS | 913 | -28.225 | -19.120 | 9.891 | 1.00 | 28.41 |
| ATOM - | 6085 | C | LYS | 913 | -27.092 | | 3.968 | | 27 40 |
| ATOM | 6086 | | | | | | | 1.00 | |
| ATOM | 0000. | | TVC | 012 | -28 156 | | | 1.00 | |
| | | 0 | LYS | 913 | | -22.656 | 4.203 | 1.00 | 37.96 |
| | 6087 | N | GLN | 914 | -26.891 | -22.656 -21.346 | 4.203 2.883 | 1.00 1.00 | 37.96 40.52 |
| MOTA | 6087 6088 | N CA | GLN | 914 914 | -26.891 -27.931 | -22.656 -21.346 -21.161 | 4.203 2.883 1.880 | 1.00 1.00 1.00 | 37.96 40.52 43.74 |
| MOTA MOTA | 6087 6088 6089 | N CA CB | GLN GLN | 914 914 914 | -26.891 -27.931 -27.498 | -22.656 -21.346 -21.161 -20.122 | 4.203 2.883 1.880 0.845 | 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 |
| MOTA | 6087 6088 | N CA | GLN | 914 914 | -26.891 -27.931 | -22.656 -21.346 -21.161 -20.122 | 4.203 2.883 1.880 | 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 |
| MOTA MOTA MOTA | 6087 6088 6089 6090 | N CA CB CG | GLN GLN GLN GLN | 914 914 914 914 | -26.891 -27.931 -27.498 | -22.656 -21.346 -21.161 -20.122 -18.745 | 4.203 2.883 1.880 0.845 1.427 | 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 |
| MOTA MOTA MOTA MOTA | 6087 6088 6089 6090 6091 | N CA CB CG CD | GLN GLN GLN GLN GLN | 914 914 914 914 914 | -26.891 -27.931 -27.498 -27.215 -26.988 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 | 4.203 2.883 1.880 0.845 1.427 0.355 | 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 |
| MOTA MOTA MOTA MOTA | 6087 6088 6089 6090 6091 6092 | N CA CB CG CD OE1 | GLN GLN GLN GLN GLN GLN | 914 914 914 914 914 914 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.405 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 | 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 |
| MOTA MOTA MOTA MOTA MOTA MOTA | 6087 6088 6089 6090 6091 6092 6093 | N CA CB CG CD OE1 NE2 | GLN GLN GLN GLN GLN GLN GLN | 914 914 914 914 914 914 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.405 -17.122 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 | 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 | N CA CB CG CD OE1 NE2 C | GLN GLN GLN GLN GLN GLN GLN GLN GLN | 914 914 914 914 914 914 914 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.405 -17.122 -22.481 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 |
| MOTA MOTA MOTA MOTA MOTA MOTA | 6087 6088 6089 6090 6091 6092 6093 | N CA CB CG CD OE1 NE2 | GLN GLN GLN GLN GLN GLN GLN | 914 914 914 914 914 914 914 914 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.405 -17.122 -22.481 -22.735 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 | N CA CB CG CD OE1 NE2 C | GLN GLN GLN GLN GLN GLN GLN GLN GLN | 914 914 914 914 914 914 914 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.405 -17.122 -22.481 -22.735 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 6095 | N CA CB CG CD OE1 NE2 C | GLN GLN GLN GLN GLN GLN GLN GLN GLN | 914 914 914 914 914 914 914 914 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.405 -17.122 -22.481 -22.735 -23.314 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 6095 6096 | N CA CB CG CD OE1 NE2 C O N | GLN GLN GLN GLN GLN GLN GLN GLN GLN | 914 914 914 914 914 914 914 914 915 915 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 -27.198 -27.327 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.405 -17.122 -22.481 -22.735 -23.314 -24.617 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 1.058 0.418 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 45.74 46.23 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 6095 6097 6098 | N CA CB CG CD OE1 NE2 C O N CA CB | GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN | 914 914 914 914 914 914 914 915 915 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 -27.198 -27.327 -26.026 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.405 -17.122 -22.481 -22.735 -23.314 -24.617 -24.988 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 1.058 0.418 -0.298 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.57 45.74 46.23 47.95 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 6095 6096 6097 6098 | N CA CB CG CD OE1 NE2 C O N CA CB | GLU GLU GLN GLN GLN GLN GLN GLN GLN GLN GLN | 914 914 914 914 914 914 914 915 915 915 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 -27.198 -27.327 -26.026 -25.516 | -22.656 -21.346 -21.161 -20.122 -17.695 -17.405 -17.122 -22.481 -22.735 -23.314 -24.617 -24.988 -23.913 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 1.058 0.418 -0.298 -1.243 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 45.74 46.23 47.95 51.08 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 6095 6096 6097 6098 6099 | N CA CB CG CD OE1 NE2 C O N CA CB CG CCD | GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU | 914 914 914 914 914 914 914 915 915 915 915 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 -27.198 -27.327 -26.026 -25.516 -24.213 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.405 -17.122 -22.481 -22.735 -23.314 -24.988 -23.913 -24.299 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 1.058 1.058 1.048 -0.298 -1.243 -1.917 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 45.74 46.23 51.08 52.26 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 6095 6096 6097 6099 6100 6101 | N CA CB CG CD OE1 NE2 C O N CA CB CG CD OE1 | GLU GLU GLU GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN | 914 914 914 914 914 914 914 915 915 915 915 915 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 -27.198 -27.327 -26.026 -24.213 -23.270 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.122 -22.481 -22.735 -23.314 -24.617 -24.988 -23.913 -24.299 -24.711 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 1.058 0.418 -0.298 -1.243 -1.917 -1.205 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 45.74 46.23 47.23 51.08 52.26 53.21 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 6095 6096 6097 6098 6100 6101 6102 | N CA CB CG CD OE1 NE2 C O N CA CB CG CD OE1 OE2 | GLU GLU GLU GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN | 914 914 914 914 914 914 914 915 915 915 915 915 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 -27.198 -27.327 -26.026 -25.516 -24.213 -24.217 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.405 -17.122 -22.481 -22.735 -23.314 -24.617 -24.988 -23.913 -24.299 -24.711 -24.181 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 1.058 0.418 -0.298 -1.243 -1.2917 -1.205 -3.157 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 45.74 46.23 47.95 51.08 52.26 53.21 53.18 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 6095 6096 6097 6099 6100 6101 | N CA CB CG CD OE1 NE2 C O N CA CB CG CD OE1 | GLU GLU GLU GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN | 914 914 914 914 914 914 914 915 915 915 915 915 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 -27.198 -27.327 -26.026 -25.516 -24.213 -23.270 -24.127 -27.654 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.405 -17.122 -22.481 -22.735 -23.314 -24.617 -24.988 -23.913 -24.299 -24.711 -24.181 -25.675 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 1.058 0.418 -0.298 -1.243 -1.917 -1.205 -3.157 1.463 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 46.23 47.95 51.08 52.26 53.21 53.18 45.27 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 6095 6096 6097 6098 6100 6101 6102 | N CA CB CG CD OE1 NE2 C O N CA CB CG CD OE1 OE2 | GLU GLU GLU GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN | 914 914 914 914 914 914 914 915 915 915 915 915 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 -27.198 -27.327 -26.026 -25.516 -24.213 -24.217 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.405 -17.122 -22.481 -22.735 -23.314 -24.617 -24.988 -23.913 -24.299 -24.711 -24.181 -25.675 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 1.058 0.418 -0.298 -1.243 -1.2917 -1.205 -3.157 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 45.74 46.23 47.95 51.08 52.26 53.21 53.18 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 6095 6096 6097 6098 6099 6100 6101 6102 6103 6104 | N CA CB CG CD OE1 NE2 C O N CA CB CG CD OE1 OE2 | GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU | 914 914 914 914 914 914 914 915 915 915 915 915 915 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 -27.198 -27.327 -26.026 -25.516 -24.213 -23.270 -24.127 -27.654 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.405 -17.122 -22.481 -22.735 -23.314 -24.988 -23.913 -24.299 -24.711 -24.181 -25.675 -26.867 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 1.058 0.418 -0.298 -1.243 -1.917 -1.205 -3.157 1.463 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 46.23 47.95 51.08 52.26 53.21 53.18 45.27 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 6095 6096 6097 6098 6099 6100 6101 6102 6103 6104 6105 | N CA CB CG CD OE1 NE2 C O N CA CB CG OE1 OE2 C O N | GLN GLN GLN GLN GLN GLN GLN GLU | 914 914 914 914 914 914 914 915 915 915 915 915 915 915 915 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 -27.198 -27.327 -26.026 -25.516 -24.213 -23.270 -24.127 -27.654 -27.700 -27.874 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.405 -17.122 -22.481 -22.735 -23.314 -24.617 -24.988 -23.913 -24.299 -24.711 -24.181 -25.675 -26.867 -25.233 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 1.058 0.418 -0.298 -1.243 -1.205 -3.157 1.463 1.160 2.697 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 45.74 46.23 47.95 51.08 52.26 53.21 53.21 53.21 54.40 94.63 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6099 6091 6092 6093 6094 6095 6096 6097 6100 6101 6102 6103 6104 6105 6106 | N CA CB CG CD OE1 NE2 C O N CA CB CG CD OE1 OE2 C O N CA CB CC O OE1 OE2 C O N CA | GLN GLN GLN GLN GLN GLN GLN GLU | 914 914 914 914 914 914 915 915 915 915 915 915 915 915 915 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 -27.198 -27.327 -26.026 -25.516 -24.213 -23.270 -24.127 -27.654 -27.700 -27.874 -28.206 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.405 -17.122 -22.481 -22.735 -23.314 -24.617 -24.988 -23.913 -24.299 -24.711 -24.181 -25.675 -26.867 -25.233 -26.138 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 1.058 1.058 -1.243 -1.291 -1.205 -3.157 1.463 1.160 2.697 3.792 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 45.74 46.23 47.95 51.08 52.26 53.21 53.18 45.27 44.09 43.28 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 6095 6096 6097 6100 6101 6102 6103 6104 6105 6106 | N CA CB CG CD OE1 NE2 C O N CA CB CG CD OE1 OE2 C O N CA CB CC C O CA CB CC | GLN GLN GLN GLN GLN GLN GLN GLN GLU | 914 914 914 914 914 914 914 915 915 915 915 915 915 915 915 916 916 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 -27.198 -27.327 -26.026 -25.516 -24.213 -23.270 -24.127 -27.654 -27.700 -27.874 -28.206 -29.587 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.405 -17.122 -22.481 -22.735 -23.314 -24.617 -24.988 -23.913 -24.299 -24.711 -24.181 -25.675 -26.867 -26.867 -25.233 -26.138 -26.754 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.418 -0.298 -1.243 -1.295 -3.157 1.463 1.160 2.697 3.792 3.558 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 45.74 46.23 47.95 51.08 52.26 53.21 53.18 45.27 45.43 44.09 43.28 45.07 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 6097 6098 6099 6100 6101 6102 6103 6104 6105 6107 6108 | N CA CB CG CD OE1 NE2 C O N CA CB CG CD OE1 OE2 C O N CA CB CG CC | GLN GLN GLN GLN GLN GLN GLN GLN GLU GLU GLU GLU GLU GLU GLU GLU LYS LYS LYS | 914 914 914 914 914 914 915 915 915 915 915 915 915 915 916 916 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 -27.198 -27.327 -26.026 -25.516 -24.213 -23.270 -24.127 -27.654 -27.700 -27.874 -27.874 -27.874 -29.587 -30.712 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.405 -17.122 -22.481 -24.617 -24.988 -23.314 -24.617 -24.988 -23.913 -24.299 -24.711 -24.181 -25.675 -26.867 -25.233 -26.754 -25.741 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 1.058 0.418 -0.298 -1.243 -1.917 -1.205 -3.157 1.463 1.160 2.697 3.792 3.558 3.545 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 45.74 46.23 47.95 51.08 52.26 53.21 53.18 45.27 45.43 44.09 43.28 45.07 46.88 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 6095 6096 6097 6098 6100 6101 6102 6103 6104 6105 6106 6107 6108 6109 | N CA CB CC O N CA CB CC O N CA CC CC C C C C C C C C C C C C C C | GLN GLN GLN GLN GLN GLN GLN GLU GLU GLU GLU GLU GLU GLU LYS LYS LYS LYS LYS | 914 914 914 914 914 914 915 915 915 915 915 915 915 916 916 916 916 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 -27.198 -27.327 -26.026 -25.516 -24.213 -23.270 -24.127 -27.654 -27.700 -27.874 -28.206 -29.587 -30.712 -30.921 | -22.656 -21.346 -21.161 -20.122 -18.745 -17.695 -17.405 -17.122 -22.481 -22.735 -23.314 -24.617 -24.988 -23.913 -24.299 -24.711 -24.181 -25.675 -26.867 -25.233 -26.754 -25.741 -25.741 -25.741 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 0.418 -0.298 -1.243 -1.917 -1.205 -3.157 1.463 1.160 2.697 3.792 3.558 3.545 4.921 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 46.23 47.95 51.08 52.26 53.21 845.27 45.43 44.99 43.28 44.50 45.63 44.50 45.64 45.64 46.88 48.53 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 6097 6098 6099 6100 6101 6102 6103 6104 6105 6107 6108 | N CA CB CG CD OE1 NE2 C O N CA CB CG CD OE1 OE2 C O N CA CB CG CC | GLN GLN GLN GLN GLN GLN GLN GLN GLU GLU GLU GLU GLU GLU GLU GLU LYS LYS LYS | 914 914 914 914 914 914 915 915 915 915 915 915 915 915 916 916 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 -27.198 -27.327 -26.026 -25.516 -24.213 -23.270 -24.127 -27.654 -27.700 -27.874 -28.206 -29.587 -30.7921 -31.908 | -22.656 -21.346 -21.161 -20.122 -17.405 -17.405 -17.122 -22.481 -22.735 -23.314 -24.988 -23.913 -24.299 -24.711 -24.181 -25.675 -26.867 -25.233 -26.138 -26.754 -25.137 -23.981 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 1.058 0.418 -0.298 -1.243 -1.217 -1.205 -3.157 1.463 1.160 2.697 3.792 3.558 3.545 4.921 4.871 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 46.23 47.95 51.08 52.26 53.21 53.21 53.21 53.21 53.21 63.21 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 6087 6088 6089 6090 6091 6092 6093 6094 6095 6096 6097 6098 6100 6101 6102 6103 6104 6105 6106 6107 6108 6109 | N CA CB CC O N CA CB CC O N CA CC CC C C C C C C C C C C C C C C | GLN GLN GLN GLN GLN GLN GLN GLU GLU GLU GLU GLU GLU GLU LYS LYS LYS LYS LYS | 914 914 914 914 914 914 915 915 915 915 915 915 916 916 916 916 | -26.891 -27.931 -27.498 -27.215 -26.988 -27.882 -25.788 -28.227 -29.357 -27.198 -27.327 -26.026 -25.516 -24.213 -23.270 -24.127 -27.654 -27.700 -27.874 -28.206 -29.587 -30.712 -30.921 | -22.656 -21.346 -21.161 -20.122 -17.405 -17.405 -17.122 -22.481 -22.735 -23.314 -24.988 -23.913 -24.299 -24.711 -24.181 -25.675 -26.867 -25.233 -26.138 -26.754 -25.137 -23.981 | 4.203 2.883 1.880 0.845 1.427 0.355 -0.442 0.327 1.183 0.768 0.418 -0.298 -1.243 -1.917 -1.205 -3.157 1.463 1.160 2.697 3.792 3.558 3.545 4.921 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 37.96 40.52 43.74 45.66 48.82 51.41 53.67 52.30 44.63 44.57 46.23 47.95 51.08 52.26 53.21 845.27 45.43 44.99 43.28 44.50 45.63 44.50 45.64 45.64 46.88 48.53 |

| ATOM | 6112 | С | LYS | 916 | -27,177 | -27.249 | 3.976 | 1.00 42.34 |
|------|-------|-----|--------|-------|--------------------|---------|------------------|------------|
| ATOM | 6113 | 0 | LYS | 916 | | -28.359 | 4.382 | 1.00 42.68 |
| ATOM | 6114 | N | LYS | 917 | | -26.949 | 3.673 | 1.00 40.67 |
| ATOM | 6115 | CA | LYS | 917 | | -27.928 | 3.823 | 1.00 38.46 |
| ATOM | 6116 | СВ | LYS | 917 | | -27.841 | 2.654 | 1.00 39.13 |
| ATOM | 6117 | CG | LYS | 917 | | -28.814 | 2.781 | 1.00 41.58 |
| ATOM | 6118 | CD | LYS | 917 | | -28.465 | 1.851 | 1.00 44.05 |
| | | | | | | | | |
| ATOM | 6119 | CE | LYS | 917 | -21.903 | | 0.387 | 1.00 46.51 |
| MOTA | 6120 | NZ | LYS | 917 | | -28.300 | -0.494 | 1.00 48.27 |
| ATOM | 6121 | C | LYS | 917 | | -27.675 | 5.123 | 1.00 36.66 |
| MOTA | 6122 | 0 | LYS | 917 | -23.297 | | 5.211 | 1.00 35.67 |
| MOTA | 6123 | N | ARG | 918 | -24.355 | | 6.129 | 1.00 33.82 |
| MOTA | 6124 | CA | ARG | 918 | -23.689 | -28.373 | 7.420 | 1.00 31.81 |
| MOTA | 6125 | CB | ARG | 918 | -24.297 | -29.362 | 8.426 | 1.00 30.96 |
| MOTA | 6126 | CG | ARG | 918 | -25.668 | -28.926 | 8.931 | 1.00 32.18 |
| ATOM | 6127 | CD | ARG | 918 | -26.346 | -29.957 | 9.826 | 1.00 33.25 |
| MOTA | 6128 | NE | ARG | 918 | -26.812 | -31.128 | 9.084 | 1.00 33.83 |
| ATOM | 6129 | CZ | ARG | 918 | -27.706 | -32.000 | 9.544 | 1.00 33.54 |
| ATOM | 6130 | NH1 | ARG | 918 | -28.240 | -31.840 | 10.747 | 1.00 33.73 |
| ATOM | 6131 | NH2 | ARG | 918 | -28.071 | -33.036 | 8.801 | 1.00 35.50 |
| ATOM | 6132 | C | ARG | 918 | -22.192 | | 7.242 | 1.00 29.61 |
| ATOM | 6133 | ō | ARG | 918 | -21.792 | | 6.557 | 1.00 29.96 |
| ATOM | 6134 | N | PHE | 919 | -21.368 | | 7.857 | 1.00 26.58 |
| ATOM | 6135 | CA | PHE | 919 | -19.911 | | 7.738 | 1.00 24.02 |
| ATOM | 6136 | CB | PHE | 919 | -19.368 | | 7.062 | 1.00 24.17 |
| ATOM | 6137 | CG | PHE | 919 | -19.743 | | 7.771 | 1.00 23.99 |
| | | | | | | | | |
| MOTA | 6138 | | PHE | 919 | -18.925 -20.932 | | 8.769 | 1.00 22.22 |
| ATOM | 6139 | | PHE | 919 | | | 7.459 | 1.00 23.20 |
| ATOM | 6140 | | PHE | 919 | -19.286 | | 9.440 | 1.00 22.28 |
| MOTA | 6141 | | PHE | 919 | -21.299 | | 8.127 | 1.00 23.01 |
| ATOM | 6142 | CZ | PHE | 919 | -20.475 | | 9.120 | 1.00 23.76 |
| ATOM | 6143 | С | PHE | 919 | -19.206 | | 9.076 | 1.00 23.65 |
| ATOM | 6144 | 0 | PHE | 919 | -19.679 | | 10.119 | 1.00 22.72 |
| ATOM | 6145 | N | ALA | 920 | -18.071 | | 9.049 | 1.00 21.57 |
| MOTA | 6146 | CA | ALA | 920 | -17.313 | | 10.276 | 1.00 19.22 |
| ATOM | 6147 | CB | ALA | 920 | -16.709 | -30.436 | 10.260 | 1.00 18.52 |
| ATOM | 6148 | C | ALA | 920 | -16.213 | -27.988 | 10.445 | 1.00 17.19 |
| ATOM | 6149 | 0 | ALA | 920 | -15.645 | -27.506 | 9.463 | 1.00 17.07 |
| ATOM | 6150 | N | THR | 921 | -15.932 | -27.644 | 11.701 | 1.00 17.33 |
| ATOM | 6151 | CA | THR | 921 | -14.904 | -26.662 | 12.071 | 1.00 17.47 |
| MOTA | 6152 | CB | THR | 921 | -15.550 | -25.358 | 12.581 | 1.00 20.30 |
| MOTA | 6153 | OG1 | THR | 921 | -16.349 | -24.781 | 11.533 | 1.00 24.13 |
| ATOM | 6154 | CG2 | THR | 921 | -14.492 | | 12.999 | 1.00 27.64 |
| MOTA | 6155 | C | THR | 921 | -14.091 | | 13.205 | 1.00 14.38 |
| ATOM | 6156 | ō. | THR | 921 | -14.586 | | 13.892 | 1.00 13.90 |
| ATOM | 6157 | N | ILE | 922 | -12.861 | | 13.424 | 1.00 13.81 |
| ATOM | 6158 | CA | ILE | 922 | -12.054 | | 14.481 | 1.00 13.01 |
| ATOM | 6159 | CB | ILE | 922 | -11.367 | | 13.943 | 1.00 15.12 |
| ATOM | 6160 | CG2 | ILE | 922 | -10.274 | | 12.925 | 1.00 15.80 |
| ATOM | 6161 | CG2 | ILE | 922 | -10.274 | | 15.102 | 1.00 15.54 |
| | 6162 | CD1 | | | -10.771 | | | 1.00 15.54 |
| | | | | 922 | | | 14.734 15.040 | |
| MOTA | 6163 | C | | 922 | -10.988 | | | 1.00 13.33 |
| ATOM | 6164 | 0 | ILE | 922 | -10.591 | | 14.375 | 1.00 13.71 |
| MOTA | 6165 | N | THR | 923 | -10.533 | | 16.262 | 1.00 13.37 |
| ATOM | 6166 | CA | THR | 923 | | -25.955 | 16.844 | 1.00 11.94 |
| MOTA | 6167 | CB | THR | 923 | | -25.979 | 18.403 | 1.00 11.46 |
| MOTA | 6168 | OG1 | THR | 923 | | -27.294 | 18.866 | 1.00 14.02 |
| MOTA | 6169 | CG2 | THR | 923 | -10.842 | | 18.962 | 1.00 12.48 |
| MOTA | 6170 | С | THR | 923 | | -26.494 | 16.358 | 1.00 11.04 |
| MOTA | 6171 | 0 | THR | 923 | | -27.662 | 15.998 | 1.00 11.93 |
| ATOM | 6172 | N | ALA | 924 | | -25.616 | 16.324 | 1.00 10.01 |
| ATOM | 6173 | CA | ALA | 924 | | -25.965 | 15.908 | 1.00 9.37 |
| MOTA | 6174 | CB | ALA | 924 | | -25.881 | 14.390 | 1.00 10.66 |
| MOTA | 6175 | С | ALA | 924 | -4.876 | -24.948 | 16.574 | 1.00 9.13 |
| MOTA | 6176 | 0 | ALA | 924 | | -23.791 | 16.738 | 1.00 9.96 |
| MOTA | 6177 | N | TYR | 925 | -3.674 | -25.367 | 16.955 | 1.00 8.67 |
| ATOM | 6178 | CA | TYR | 925 | -2.757 | -24.463 | 17.638 | 1.00 10.02 |
| MOTA | 6179 | СВ | TYR | 925 | | -24.709 | 19.143 | 1.00 9.74 |
| ATOM | 6180 | CG | TYR | 925 | | -25.007 | 19.687 | 1.00 10.81 |
| ATOM | 6181 | CD1 | TYR | 925 | | -26.328 | 19.842 | 1.00 11.73 |
| ATOM | 6182 | CE1 | TYR | 925 | | -26.625 | 20.373 | 1.00 12.92 |
| ATOM | 6183 | | TYR | 925 | | -23.982 | 20.069 | 1.00 11.21 |
| ATOM | 6184 | CE2 | TYR | 925 | | -24.269 | 20.603 | 1.00 10.91 |
| ATOM | 6185 | CZ | TYR | 925 | | -25.592 | 20.752 | 1.00 12.01 |
| ATOM | 6186 | OH | TYR | 925 | | -25.890 | 21.293 | 1.00 13.23 |
| ATOM | 6187 | C | TYR | 925 | | -24.619 | 17.174 | 1.00 13.23 |
| ATOM | 6188 | 0 | TYR | 925 | | -24.013 | 17.744 | 1.00 10.90 |
| 011 | 0.100 | _ | T T T/ | , , , | J. 42 U | VI/ | _ , , , == | 10.70 |

| ATOM | 6189 | N | ASP | 926 | -1.106 | -25.447 | 16.161 | 1.00 8.96 |
|--------|------|-----|-----|-----|--------|---------|--------|--------------------------|
| ATOM | 6190 | CA | ASP | 926 | 0.250 | -25.626 | 15.672 | 1.00 10.92 |
| ATOM | 6191 | СВ | ASP | 926 | 0.971 | -26.694 | 16.509 | 1.00 11.44 |
| ATOM | 6192 | CG | ASP | 926 | 0.378 | -28.093 | 16.328 | 1.00 11.32 |
| ATOM | 6193 | | ASP | 926 | 0.546 | -28.668 | 15.247 | 1.00 11.50 |
| ATOM | 6194 | OD2 | ASP | 926 | | -28.601 | 17.274 | 1.00 15.55 |
| ATOM | 6195 | C | ASP | 926 | | -25.982 | 14.186 | 1.00 11.52 |
| ATOM | | 0 | ASP | 926 | | -26.292 | 13.581 | 1.00 13.19 |
| | 6196 | | | | | | 13.610 | |
| ATOM | 6197 | N | TYR | 927 | | -25.929 | | 1.00 9.04 |
| MOTA | 6198 | CA | TYR | 927 | 1.693 | -26.206 | 12.190 | 1.00 9.91 |
| MOTA | 6199 | CB | TYR | 927 | 3.183 | -26.037 | 11.848 | 1.00 12.47 |
| MOTA | 6200 | CG | TYR | 927 | | -26.566 | 10.486 | 1.00 13.30 |
| MOTA | 6201 | CD1 | | 927 | | -25.805 | 9.332 | 1.00 15.77 |
| MOTA | 6202 | CE1 | TYR | 927 | | -26.286 | 8.072 | 1.00 17.93 |
| MOTA | 6203 | CD2 | TYR | 927 | 4.175 | -27.831 | 10.351 | 1.00 14.44 |
| MOTA | 6204 | CE2 | TYR | 927 | 4.548 | -28.327 | 9.092 | 1.00 15.72 |
| ATOM | 6205 | cz | TYR | 927 | 4.345 | -27.552 | 7.961 | 1.00 18.75 |
| ATOM | 6206 | ОН | TYR | 927 | 4.694 | -28.034 | 6.708 | 1.00 20.14 |
| ATOM | 6207 | С | TYR | 927 | | -27.588 | 11.745 | 1.00 12.26 |
| MOTA | 6208 | ō | TYR | 927 | | -27.732 | 10.791 | 1.00 12.34 |
| ATOM | 6209 | N | SER | 928 | | -28.602 | 12.446 | 1.00 11.45 |
| ATOM | 6210 | CA | SER | 928 | 1.468 | -29.987 | 12.097 | 1.00 11.62 |
| | 6211 | CB | SER | 928 | | -30.928 | 13.077 | 1.00 12.06 |
| MOTA | | | SER | | | | | |
| ATOM | 6212 | OG | | 928 | | -30.869 | 12.883 | 1.00 14.47 |
| MOTA | 6213 | C | SER | 928 | | -30.361 | 11.990 | 1.00 11.37 |
| ATOM | 6214 | 0 | SER | 928 | | -30.992 | 11.008 | 1.00 11.30 |
| MOTA | 6215 | N | PHE | 929 | | -30.004 | 12.997 | 1.00 10.21 |
| MOTA | 6216 | CA | PHE | 929 | | -30.337 | 12.932 | 1.00 9.78 |
| MOTA | 6217 | CB | PHE | 929 | -2.852 | -30.267 | 14.319 | 1.00 11.80 |
| MOTA | 6218 | CG | PHE | 929 | -2.628 | -31.504 | 15.132 | 1.00 10.16 |
| MOTA | 6219 | CD1 | PHE | 929 | -1.601 | -31.570 | 16.063 | 1.00 9.07 |
| ATOM . | 6220 | CD2 | PHE | 929 | -3.383 | -32.645 | 14.879 | 1.00 13.10 |
| ATOM | 6221 | CE1 | PHE | 929 | -1.325 | -32.766 | 16.737 | 1.00 11.64 |
| ATOM | 6222 | CE2 | PHE | 929 | -3.122 | -33.838 | 15.539 | 1.00 10.99 |
| ATOM | 6223 | CZ | PHE | 929 | -2.092 | -33.903 | 16.465 | 1.00 10.50 |
| ATOM | 6224 | C | PHE | 929 | | -29.479 | 11.935 | 1.00 10.59 |
| ATOM | 6225 | 0 | PHE | 929 | | -29.970 | 11.280 | 1.00 10.30 |
| | 6226 | | ALA | 930 | | -28.210 | 11.798 | 1.00 10.20 |
| | | N | | | | | | |
| ATOM | 6227 | CA | ALA | 930 | | -27.341 | 10.835 | 1.00 10.49 |
| MOTA | 6228 | CB | ALA | 930 | | -25.899 | 10.940 | 1.00 10.94 |
| ATOM | 6229 | C | ALA | 930 | | -27.891 | 9.427 | 1.00 11.83 |
| MOTA | 6230 | О | ALA | 930 | | -27.870 | 8.572 | 1.00 12.93 |
| MOTA | 6231 | N | LYS | 931 | | -28.361 | 9.192 | 1.00 11.22 |
| MOTA | 6232 | CA | LYS | 931 | -1.425 | -28.924 | 7.894 | 1.00 12.92 |
| ATOM | 6233 | CB | LYS | 931 | 0.078 | -29.232 | 7.897 | 1.00 13.90 |
| MOTA | 6234 | CG | LYS | 931 | 0.628 | -29.953 | 6.669 | 1.00 19.23 |
| ATOM | 6235 | CD | LYS | 931 | 0.716 | -29.053 | 5.467 | 1.00 22.53 |
| ATOM | 6236 | CE | LYS | 931 | | -29.628 | 4.415 | 1.00 26.66 |
| ATOM | 6237 | NZ | LYS | 931 | | -30.976 | 3.915 | 1.00 26.76 |
| ATOM | 6238 | C | LYS | 931 | | -30.198 | 7.646 | 1.00 12.48 |
| ATOM | 6239 | 0 | LYS | 931 | | -30.428 | 6.543 | 1.00 14.08 |
| • | 6240 | Ŋ | LEU | 932 | | -31.029 | 8.672 | 1.00 11.21 |
| MOTA | | | | | | | | |
| ATOM | 6241 | CA | LEU | 932 | | -32.273 | 8.557 | 1.00 11.84 1.00 11.17 |
| ATOM | 6242 | CB | LEU | 932 | | -33.060 | 9.865 | |
| ATOM | 6243 | CG | LEU | 932 | | -34.485 | 9.854 | 1.00 11.63 |
| ATOM | 6244 | CD1 | | 932 | | -35.309 | 10.946 | 1.00 10.37 |
| ATOM | 6245 | CD2 | | 932 | | -34.430 | 10.059 | 1.00 12.21 |
| MOTA | 6246 | С | | 932 | | -31.991 | 8.212 | 1.00 12.85 |
| MOTA | 6247 | 0 | LEU | 932 | | -32.611 | 7.309 | 1.00 14.20 |
| MOTA | 6248 | N | PHE | 933 | -5.140 | -31.039 | 8.913 | 1.00 12.43 |
| MOTA | 6249 | CA | PHE | 933 | -6.538 | -30.699 | 8.663 | 1.00 12.70 |
| MOTA | 6250 | CB | PHE | 933 | -7.036 | -29.670 | 9.691 | 1.00 12.30 |
| MOTA | 6251 | CG | PHE | 933 | -6.939 | -30.139 | 11.120 | 1.00 10.75 |
| MOTA | 6252 | CD1 | | 933 | | -31.493 | 11.430 | 1.00 11.83 |
| ATOM | 6253 | CD2 | | 933 | | -29.224 | 12.162 | 1.00 11.03 |
| ATOM | 6254 | CE1 | | 933 | | -31.931 | 12.744 | 1.00 11.61 |
| ATOM | 6255 | | PHE | 933 | -6.699 | | 13.482 | 1.00 11.00 |
| ATOM | 6256 | CZ | PHE | 933 | | -31.014 | 13.774 | 1.00 12.40 |
| | | | | | | | | |
| MOTA | 6257 | С | PHE | 933 | | -30.174 | 7.247 | 1.00 14.52 |
| ATOM | 6258 | 0 | PHE | 933 | | -30.661 | 6.551 | 1.00 14.70 |
| ATOM | 6259 | N | ALA | 934 | | -29.181 | 6.822 | 1.00 14.17 |
| ATOM | 6260 | CA | ALA | 934 | | -28.607 | 5.488 | 1.00 16.25 |
| ATOM | 6261 | CB | ALA | 934 | | -27.499 | 5.266 | 1.00 15.86 |
| MOTA | 6262 | С | ALA | 934 | | -29.661 | 4.397 | 1.00 18.38 |
| MOTA | 6263 | 0 | ALA | 934 | -6.742 | -29.631 | 3.399 | 1.00 19.61 |
| MOTA | 6264 | N | ASP | 935 | -5.094 | -30.585 | 4.586 | 1.00 18.37 |
| ATOM | 6265 | CA | ASP | 935 | -4.873 | -31.632 | 3.605 | 1.00 20.68 |
| | | | | | | | | |

| ATOM 6267 CG ASP 935 -2.341 -31.618 3.716 ATOM 6268 OD1 ASP 935 -2.426 -30.459 3.253 ATOM 6269 OD2 ASP 935 -1.256 -32.155 4.001 ATOM 6270 C ASP 935 -6.050 -32.588 3.492 ATOM 6271 O ASP 935 -6.152 -33.332 2.518 ATOM 6272 N GLU 936 -6.937 -32.570 4.481 ATOM 6273 CA GLU 936 -8.107 -33.449 4.466 | 1.00 22.05 1.00 24.26 1.00 28.99 1.00 24.81 1.00 21.54 |
|--|--|
| ATOM 6267 CG ASP 935 -2.341 -31.618 3.716 ATOM 6268 OD1 ASP 935 -2.426 -30.459 3.253 ATOM 6269 OD2 ASP 935 -1.256 -32.155 4.001 ATOM 6270 C ASP 935 -6.050 -32.588 3.492 ATOM 6271 O ASP 935 -6.152 -33.332 2.518 ATOM 6272 N GLU 936 -6.937 -32.570 4.481 ATOM 6273 CA GLU 936 -8.107 -33.449 4.466 | 1.00 28.99 1.00 24.81 |
| ATOM 6268 OD1 ASP 935 -2.426 -30.459 3.253 ATOM 6269 OD2 ASP 935 -1.256 -32.155 4.001 ATOM 6270 C ASP 935 -6.050 -32.588 3.492 ATOM 6271 O ASP 935 -6.152 -33.332 2.518 ATOM 6272 N GLU 936 -6.937 -32.570 4.481 ATOM 6273 CA GLU 936 -8.107 -33.449 4.466 | 1.00 24.81 |
| ATOM 6269 OD2 ASP 935 -1.256 -32.155 4.001 ATOM 6270 C ASP 935 -6.050 -32.588 3.492 ATOM 6271 O ASP 935 -6.152 -33.332 2.518 ATOM 6272 N GLU 936 -6.937 -32.570 4.481 ATOM 6273 CA GLU 936 -8.107 -33.449 4.466 | 1.00 24.81 |
| ATOM 6270 C ASP 935 -6.050 -32.588 3.492 ATOM 6271 O ASP 935 -6.152 -33.332 2.518 ATOM 6272 N GLU 936 -6.937 -32.570 4.481 ATOM 6273 CA GLU 936 -8.107 -33.449 4.466 | |
| ATOM 6271 O ASP 935 -6.152 -33.332 2.518 ATOM 6272 N GLU 936 -6.937 -32.570 4.481 ATOM 6273 CA GLU 936 -8.107 -33.449 4.466 | |
| ATOM 6272 N GLU 936 -6.937 -32.570 4.481 ATOM 6273 CA GLU 936 -8.107 -33.449 4.466 | 1.00 21.57 |
| ATOM 6273 CA GLU 936 -8.107 -33.449 4.466 | 1.00 21.37 |
| | |
| ATOM 6274 CB GLU 936 -8.300 -34.119 5.830 | 1.00 23.46 |
| | 1.00 22.13 |
| | 1.00 25.30 |
| ATOM 6276 CD GLU 936 -6.944 -36.134 5.184 | 1.00 26.05 |
| ATOM 6277 OE1 GLU 936 -7.932 -36.697 4.664 | 1.00 27.53 |
| ATOM 6278 OE2 GLU 936 -5.768 -36.408 4.890 | 1.00 25.51 |
| ATOM 6279 C GLU 936 -9.395 -32.727 4.090 | 1.00 23.90 |
| | 1.00 23.71 |
| | 1.00 24.48 |
| 111011 0101 11 011 | 1.00 24.58 |
| | 1.00 24.70 |
| | |
| | 1.00 22.63 |
| | 1.00 21.96 |
| | 1.00 22.24 |
| | 1.00 22.44 |
| ATOM 6288 CG LEU 938 -11.881 -30.305 9.325 | 1.00 24.89 |
| ATOM 6289 CD1 LEU 938 -11.300 -30.960 10.565 | 1.00 20.46 |
| ATOM 6290 CD2 LEU 938 -12.736 -29.116 9.706 | 1.00 23.65 |
| | 1.00 22.22 |
| | 1.00 21.13 |
| | 1.00 19.30 |
| | 1.00 20.12 |
| | |
| | 1.00 21.00 |
| | 1.00 24.01 |
| | 1.00 24.14 |
| | 1.00 24.93 |
| ATOM 6299 C ASN 939 -10.959 -24.393 7.000 | 1.00 17.21 |
| ATOM 6300 O ASN 939 -10.813 -23.234 6.631 | 1.00 17.54 |
| ATOM 6301 N VAL 940 -11.564 -24.705 8.139 | 1.00 15.30 |
| | 1.00 12.98 |
| | 1.00 13.67 |
| | 1.00 14.67 |
| | 1.00 15.61 |
| | 1.00 13.01 |
| | 1.00 12.24 |
| | |
| | 1.00 11.66 |
| | 1.00 11.33 |
| | 1.00 11.01 |
| | 1.00 15.14 |
| ATOM 6312 SD MET 941 -6.605 -25.492 10.723 | 1.00 13.23 |
| ATOM 6313 CE MET 941 -6.628 -25.995 9.032 | 1.00 16.00 |
| ATOM 6314 C MET 941 -9.935 -22.338 13.136 | 1.00 11.83 |
| | 1.00 12.66 |
| | 1.00 10.99 |
| | 1.00 12.19 |
| | 1.00 15.75 |
| | 1.00 20.87 |
| | |
| | 1.00 25.90 |
| | 1.00 18.03 |
| | 1.00 12.22 |
| • | 1.00 11.14 |
| ATOM 6324 N VAL 943 -8.160 -20.728 16.528 | 1.00 11.13 |
| ATOM 6325 CA VAL 943 -7.048 -20.703 17.464 | 1.00 10.52 |
| ATOM 6326 CB VAL 943 -5.889 -19.821 16.965 | 1.00 10.69 |
| | 1.00 11.40 |
| | 1.00 13.59 |
| | 1.00 11.08 |
| | 1.00 11.38 |
| | 1.00 13.26 |
| | 1.00 13.26 |
| | |
| | 1.00 11.45 |
| | 1.00 11.27 |
| | 1.00 10.87 |
| | 1.00 11.19 |
| ATOM 6337 CB ASP 945 -8.602 -18.519 25.103 | 1.00 12.8,4 |
| | 1.00 15.40 |
| | 1.00 14.02 |
| | 1.00 16.56 |
| AIVE 0340 UUX ASE 343 -10.012 -17.344 23.888 | 1.00 10.85 |
| | |
| ATOM 6341 C ASP 945 -8.216 -21.021 25.034 | 1.00 11.48 |

| ATOM | 6343 | N | SER | 946 | | -8.829 | -22.019 | 24.392 | 1.00 10.80 |
|------|-------|-----|-------|-----|---|----------|---------|--------|------------|
| ATOM | 6344 | CA | SER | 946 | | -8.929 | -23.346 | 25.000 | 1.00 11.18 |
| ATOM | 6345 | СВ | SER | 946 | | | -24.282 | 24.109 | 1.00 13.04 |
| ATOM | 6346 | ŌĞ | SER | 946 | | | -24.167 | 22.750 | 1.00 13.51 |
| ATOM | 6347 | c | SER | 946 | | | -23.841 | 25.098 | 1.00 12.33 |
| | 6348 | ō | SER | 946 | | | -24.746 | 25.878 | 1.00 12.87 |
| ATOM | | | | | | | | | |
| MOTA | 6349 | N | LEU | 947 | | | -23.241 | 24.292 | 1.00 9.71 |
| ATOM | 6350 | CA | LEU | 947 | | | -23.620 | 24.319 | 1.00 10.28 |
| ATOM | 6351 | CB | LEU | 947 | | | -22.834 | 23.260 | 1.00 9.98 |
| MOTA | 6352 | CG | LEU | 947 | | | -21.308 | 23.369 | 1.00 10.69 |
| MOTA | 6353 | CD1 | LEU | 947 | | -3.110 | -20.959 | 24.301 | 1.00 10.73 |
| ATOM | 6354 | CD2 | LEU | 947 | | -3.955 | -20.712 | 21.980 | 1.00 11.38 |
| ATOM | 6355 | С | LEU | 947 | | -4.607 | -23.391 | 25.717 | 1.00 9.28 |
| ATOM | 6356 | 0 | LEU | 947 | | -3.627 | -24.038 | 26.114 | 1.00 10.82 |
| ATOM | 6357 | N | GLY | 948 | | | -22.474 | 26.468 | 1.00 9.77 |
| ATOM | 6358 | CA | GLY | 948 | | | -22.208 | 27.819 | 1.00 9.51 |
| ATOM | 6359 | C | GLY | 948 | | | -23.482 | 28.651 | 1.00 10.76 |
| | 6360 | 0 | GLY | 948 | | | -23.647 | 29.570 | 1.00 10.19 |
| ATOM | | | | | | | | | |
| MOTA | 6361 | N | MET | 949 | | | -24.389 | 28.325 | 1.00 10.94 |
| ATOM | 6362 | CA | MET | 949 | | | -25.637 | 29.063 | 1.00 12.90 |
| ATOM | 6363 | CB | MET | 949 | | | -25.952 | 29.349 | 1.00 12.40 |
| ATOM | 6364 | CG | MET | 949 | | | -24.849 | 30.130 | 1.00 15.92 |
| MOTA | 6365 | SD | MET | 949 | | -9.725 | -25.184 | 30.491 | 1.00 22.24 |
| MOTA | 6366 | CE | MET | 949 | | -9.565 | -26.325 | 31.869 | 1.00 23.74 |
| MOTA | 6367 | С | MET | 949 | | -5.153 | -26.794 | 28.313 | 1.00 13.79 |
| ATOM | 6368 | 0 | MET | 949 | | -4.272 | -27.473 | 28.840 | 1.00 13.01 |
| ATOM | 6369 | N | THR | 950 | | | -27.003 | 27.072 | 1.00 13.13 |
| ATOM | 6370 | CA | THR | 950 | | | -28.104 | 26.271 | 1.00 14.84 |
| ATOM | 6371 | CB | THR | 950 | | | -28.243 | 24.975 | 1.00 18.87 |
| | | | | | | | -29.536 | 24.407 | 1.00 27.10 |
| MOTA | 6372 | OG1 | THR | 950 | | | | | |
| MOTA | 6373 | CG2 | THR | 950 | | | -27.177 | 23.971 | 1.00 15.75 |
| ATOM | 6374 | С | THR | 950 | | | -28.027 | 25.922 | 1.00 14.92 |
| MOTA | 6375 | Ο, | THR | 950 | | -2.887 | -29.053 | 25.875 | 1.00 14.14 |
| ATOM | 6376 | N | VAL | 951 | | -3.064 | -26.819 | 25.688 | 1.00 12.91 |
| MOTA | 6377 | CA | VAL | 951 | | -1.663 | -26.639 | 25.330 | 1.00 12.41 |
| MOTA | 6378 | CB | VAL | 951 | | -1.532 | -25.597 | 24.174 | 1.00 13.11 |
| ATOM | 6379 | CG1 | VAL | 951 | | -0.074 | -25.297 | 23.888 | 1.00 13.39 |
| ATOM | 6380 | | VAL | 951 | | | -26.131 | 22.918 | 1.00 13.74 |
| ATOM | 6381 | C | VAL | 951 | | | -26.213 | 26.502 | 1.00 12.91 |
| ATOM | 6382 | ō | VAL | 951 | | | -26.855 | 26.782 | 1.00 13.09 |
| | 6383 | N | GLN | 952 | | | -25.138 | 27.190 | 1.00 10.78 |
| ATOM | | | | | | | -23.136 | | |
| ATOM | 6384 | CA | GLN | 952 | | | | 28.312 | 1.00 12.90 |
| ATOM | 6385 | CB | GLN | 952 | | | -23.149 | 28.540 | 1.00 9.47 |
| ATOM | 6386 | CG | GLN . | 952 | | | -22.295 | 27.299 | 1.00, 1022 |
| MOTA | 6387 | CD | GLN | 952 | | | -20.862 | 27.509 | 1.00 10.55 |
| MOTA | 6388 | OE1 | GLN | 952 | | -1.485 | -20.527 | 28.523 | 1.00 11.30 |
| ATOM | 6389 | NE2 | GLN | 952 | | -0.571 | -20.006 | 26.547 | 1.00 6.63 |
| ATOM | 6390 | С | GLN | 952 | | -0.534 | -25.385 | 29.628 | 1.00 12.56 |
| ATOM | 6391 | 0 | GLN | 952 | | 0.327 | -25.319 | 30.503 | 1.00 14.66 |
| ATOM | 6392 | N | GLY | 953 | | -1.667 | -26.061 | 29.791 | 1.00 12.38 |
| ATOM | 6393 | CA | GLY | 953 | | | -26.821 | 31.009 | 1.00 12.40 |
| ATOM | 6394 | C | GLY | 953 | | | -26.083 | 32.206 | 1.00 12.68 |
| | 6395 | 0 | | 953 | | | -26.531 | 33.344 | 1.00 12.00 |
| ATOM | 6396 | | GLY | | | | -24.953 | 31.971 | 1.00 13.33 |
| ATOM | | N | HIS | 954 | | | | 33.067 | |
| ATOM | 6397 | CA | HIS | 954 | | | -24.206 | | 1.00 12.78 |
| ATOM | 6398 | CB | HIS | 954 | | | -22.731 | 32.700 | 1.00 11.26 |
| ATOM | 6399 | CG | HIS | 954 | | | -22.013 | 32.546 | 1.00 13.33 |
| MOTA | 6400 | | HIS | 954 | | | -21.430 | | 1.00 13.37 |
| MOTA | 6401 | ND1 | HIS | 954 | | -1.706 | -21.852 | 33.591 | 1.00 13.34 |
| ATOM | 6402 | CE1 | HIS | 954 | | -0.640 | -21.200 | 33.165 | 1.00 15.92 |
| MOTA | 6403 | NE2 | HIS | 954 | | -0.801 | -20.931 | 31.882 | 1.00 13.61 |
| ATOM | 6404 | С | HIS | 954 | | -5.083 | -24.814 | 33.357 | 1.00 13.36 |
| ATOM | 6405 | 0 | HIS | 954 | | | -25.594 | 32.555 | 1.00 13.27 |
| ATOM | 6406 | N | ASP | 955 | | | -24.458 | 34.511 | 1.00 16.24 |
| ATOM | 6407 | CA | ASP | 955 | | | -24.963 | 34.944 | 1.00 10.24 |
| ATOM | 6408 | CB | ASP | 955 | | | -24.882 | 36.473 | 1.00 23.17 |
| | | | | | | | | | 1.00 23.17 |
| ATOM | 6409 | CG | ASP | 955 | • | | -23.457 | 36.998 | |
| | 6410 | | ASP | 955 | | | -22.566 | 36.495 | 1.00 31.02 |
| MOTA | 6411 | | ASP | 955 | | | -23.231 | 37.932 | 1.00 32.90 |
| ATOM | 6412 | С | ASP | 955 | | | -24.221 | 34.315 | 1.00 17.97 |
| ATOM | 6413 | 0 | ASP | 955 | | | -24.605 | 34.493 | 1.00 16.08 |
| MOTA | 6414 | N | SER | 956 | | -7.825 | -23.151 | 33.593 | 1.00 15.35 |
| ATOM | 6415 | CA | SER | 956 | | -8.845 | -22.364 | 32.926 | 1.00 14.44 |
| ATOM | 6416 | СВ | SER | 956 | | | -21.320 | 33.878 | 1.00 14.03 |
| ATOM | 6417 | OG | SER | 956 | | | -20.269 | 34.155 | 1.00 12.64 |
| ATOM | 6418 | c | SER | 956 | | | -21.676 | 31.732 | 1.00 13.94 |
| ATOM | 6419 | 0 | SER | 956 | | | -21.806 | 31.517 | 1.00 12.60 |
| 0+1 | 0-317 | _ | | 200 | | 2.,,,,,, | | , | |

| ATOM | 6420 | N | THR | 957 | -8.997 | -20.955 | 30.953 | 1.00 12.70 |
|--------------|--------------|------------|------|------------|---------|--------------------|------------------|-------------------------|
| ATOM | 6421 | CA | THR | 957 | -8.495 | -20.259 | 29.774 | 1.00 11.18 |
| ATOM | 6422 | CB | THR | 957 | | -20.165 | 28.690 | 1.00 10.23 |
| ATOM | 6423 | | THR | 957 | -10.710 | | 29.217 | 1.00 12.66 |
| ATOM | 6424 | CG2 | THR | 957 | -10.017 | | 28.231 | 1.00 13.69 |
| ATOM | 6425 | C | THR | 957 | | -18.834 | 30.114 | 1.00 10.60 |
| ATOM | 6426 | ō | THR | 957 | | -18.164 | 29.295 | 1.00 9.48 |
| ATOM | 6427 | N | LEU | 958 | | -18.371 | 31.318 | 1.00 11.09 |
| ATOM | 6428 | CA | LEU | 958 | | -16.999 | 31.718 | 1.00 10.38 |
| ATOM | 6429 | CB | LEU | 958 | | -16.756 | 33.167 | 1.00 11.85 |
| ATOM | 6430 | CG | LEU | 958 | | -16.399 | 33.380 | 1.00 14.28 |
| ATOM | 6431 | | LEU | 958 | | -17.587 | 33.066 | 1.00 13.28 |
| ATOM | 6432 | | LEU | 958 | -10.159 | | 34.824 | 1.00 16.63 |
| ATOM | 6433 | C | LEU | 958 | | -16.545 | 31.525 | 1.00 10.13 |
| ATOM | 6434 | ō | LEU | 958 | | -15.413 | 31.106 | 1.00 10.74 |
| ATOM | 6435 | N | PRO | 959 | | -17.417 | 31.819 | 1.00 11.82 |
| ATOM | 6436 | CD | PRO | 959 | | -18.691 | 32.549 | 1.00 12.19 |
| ATOM | 6437 | CA | PRO | 959 | | -17.015 | 31.645 | 1.00 10.66 |
| ATOM | 6438 | CB | PRO | 959 | | -18.170 | 32.284 | 1.00 13.42 |
| ATOM | 6439 | CG | PRO | 959 | | -19.328 | 32.170 | 1.00 19.51 |
| ATOM | 6440 | C | PRO | 959 | | -16.711 | 30.225 | 1.00 10.61 |
| ATOM | 6441 | 0 | PRO | 959 | | -16.086 | 30.054 | 1.00 9.35 |
| ATOM | 6442 | N | VAL | 960 | | -17.139 | 29.214 | 1.00 10.44 |
| ATOM | 6443 | CA | VAL | 960 | | -16.924 | 27.821 | 1.00 10.44 |
| ATOM | 6444 | CB | VAL | 960 | | -17.647 | 26.858 | 1.00 10.31 |
| ATOM | 6445 | | VAL | 960 | | -17.492 | 25.408 | 1.00 10.31 |
| ATOM | 6446 | CG2 | | 960 | | -19.116 | 27.212 | 1.00 10.51 |
| | | C | ·VAL | 960 | | -15.455 | 27.455 | 1.00 10.51 |
| ATOM ATOM | 6448 | 0 | VAL | 960 | | -14.723 | 27.433 | 1.00 11.03 |
| ATOM | 6449 | N | THR | 961 | | -15.012 | 26.917 | 1.00 11.69 |
| ATOM | 6450 | CA | THR | 961 | | -13.610 | 26.553 | 1.00 12.59 |
| ATOM | 6451 | CB | THR | 961 | | -12.975 | 27.142 | 1.00 16.60 |
| ATOM | 6452 | OG1 | | 961 | | -13.392 | 28.510 | 1.00 22.57 |
| ATOM | 6453 | CG2 | THR | 961 | | -11.461 | 27.095 | 1.00 22.84 |
| ATOM | 6454 | C | THR | 961 | | -13.423 | 25.040 | 1.00 11.62 |
| ATOM | 6455 | ō | THR | 961 | | -14.393 | 24.272 | 1.00 8.55 |
| ATOM | 6456 | N | VAL | 962 | | -12.171 | 24.613 | 1.00 8.97 |
| ATOM | 6457 | CA | VAL | 962 | | -11.870 | 23.189 | 1.00 9.43 |
| ATOM | 6458 | CB | VAL | 962 | -3.205 | -10.344 | 22.954 | 1.00 12.17 |
| MOTA | 6459 | CG1 | VAL | 962 | -3.243 | -10.044 | 21.457 | 1.00 9.65 |
| ATOM | 6460 | CG2 | VAL | 962 | -4.464 | -9.842 | 23.640 | 1.00 15.11 |
| ATOM | 6461 | С | VAL | 962 | -1.813 | -12.390 | 22.486 | 1.00 10.49 |
| ATOM | 6462 | 0 | VAL | 962 | -1.902 | -13.023 | 21.434 | 1.00 10.98 |
| MOTA | 6463 | N | ALA | 963 | -0.650 | -12.142 | 23.080 | 1.00 9.85 |
| MOTA | 6464 | CA | ALA | 963 | | -12.604 | 22.489 | 1.00 10.83 |
| ATOM | 6465 | CB | ALA | 963 | | -12.235 | 23.397 | 1.00 10.40 |
| MOTA | 6466 | С | ALA | 963 | | -14.120 | 22.258 | 1.00 10.40 |
| ATOM | 6467 | 0 | ALA | 963 | | -14.593 | 21.256 | 1.00 10.00 |
| MOTA | 6468 | N | ASP | 964 | | -14.866 | | 1.00 12.44 |
| MOTA | 6469 | CA | ASP | 964 | | -16.326 | 23.067 | 1.00 11.54 |
| MOTA | 6470 | CB | ASP | 964 | | -16.961 | 24.289 | 1.00 11.14 |
| ATOM | 6471 | CG | ASP | 964 | | -16.816 | 25.572 | 1.00 13.23 |
| ATOM | 6472 | OD1 | | 964 | | -16.781 | 25.528 | 1.00 11.81 |
| ATOM | 6473 | OD2 | | 964 | | -16.761 | 26.648 | 1.00 12.48 |
| ATOM | 6474 | С | ASP | 964 | | -16.692 | 21.833 | 1.00 11.21 1.00 6.94 |
| ATOM | 6475 | 0 | ASP | 964 | | -17.561 | 21.048 21.680 | |
| ATOM | 6476 | N | ILE | 965 | | -16.037 | | 1.00 8.84 1.00 9.08 |
| ATOM | 6477 | CA | ILE | 965 | | -16.292 -15.435 | 20.539 | 1.00 9.08 1.00 9.58 |
| ATOM | 6478 | CB | ILE | 965 965 | | -15.617 | 20.593 19.298 | 1.00 7.50 |
| ATOM ATOM | 6479 6480 | CG2 CG1 | | 965 | | -15.814 | 21.813 | 1.00 7.30 |
| ATOM | 6481 | CD1 | | 965 | | -17.185 | 21.739 | 1.00 9.87 |
| ATOM | 6482 | CDI | ILE | 965 | | -15.970 | 19.244 | 1.00 9.13 |
| ATOM | 6483 | 0 | ILE | 965 | | -16.725 | 18.267 | 1.00 8.12 |
| ATOM | 6484 | N | ALA | 966 | | -14.851 | 19.231 | 1.00 9.33 |
| ATOM | 6485 | CA | ALA | 966 | | -14.453 | 18.026 | 1.00 7.88 |
| ATOM | 6486 | CB | ALA | 966 | | -13.046 | 18.215 | 1.00 10.51 |
| ATOM | 6487 | C | ALA | 966 | | -15.459 | 17.665 | 1.00 6.25 |
| ATOM | 6488 | ō | ALA | 966 | | -15.694 | 16.484 | 1.00 8.05 |
| АТОМ | 6489 | N | TYR | 967 | | -16.023 | 18.690 | 1.00 7.24 |
| MOTA | 6490 | CA | TYR | 967 | | -17.022 | 18.487 | 1.00 7.41 |
| MOTA | 6491 | СВ | TYR | 967 | | -17.433 | 19.847 | 1.00 8.25 |
| ATOM | 6492 | CG | TYR | 967 | | -18.579 | 19.775 | 1.00 9.15 |
| ATOM | 6493 | CD1 | | 967 | 4.858 | -18.406 | 19.191 | 1.00 10.05 |
| ATOM | 6494 | CE1 | TYR | 967 | | -19.444 | 19.151 | 1.00 12.77 |
| ATOM | 6495 | CD2 | TYR | 967 | | -19.826 | 20.314 | 1.00 9.48 |
| MOTA | 6496 | CE2 | TYR | 967 | 4.217 | -20.876 | 20.278 | 1.00 13.60 |

| ATOM | 6497 | CZ | TYR | 967 | 5.462 | -20.673 | 19.695 | 1.00 | 13.29 |
|--------|-------|-----|-------|-----|--------|-----------|--------|------|-------|
| ATOM | 6498 | OH | TYR | 967 | 6.394 | -21.697 | 19.655 | 1.00 | 13.05 |
| ATOM | 6499 | C | TYR | 967 | | -18.266 | 17.772 | 1.00 | 6.51 |
| ATOM | 6500 | 0 | TYR | 967 | | -18.745 | 16.776 | 1.00 | 5.94 |
| | | | | 968 | | -18.783 | 18.296 | 1.00 | 9.58 |
| ATOM | 6501 | N | HIS | | | | | | |
| MOTA | 6502 | CA | HIS | 968 | | -19.994 | 17.741 | 1.00 | 9.37 |
| MOTA | 6503 | CB | HIS | 968 | | -20.593 | 18.784 | 1.00 | 8.45 |
| ATOM | 6504 | CG | HIS | 968 | | -21.162 | 19.988 | 1.00 | 9.03 |
| MOTA | 6505 | CD2 | HIS | 968 | | -20.670 | 21.241 | 1.00 | 8.58 |
| ATOM | 6506 | ND1 | HIS | 968 | 0.147 | -22.360 | 19.954 | 1.00 | 8.08 |
| ATOM | 6507 | CE1 | HIS | 968 | 0.714 | -22.582 | 21.129 | 1.00 | 9.22 |
| ATOM | 6508 | NE2 | HIS | 968 | 0.424 | -21.573 | 21.929 | 1.00 | 7.98 |
| ATOM | 6509 | С | HIS | 968 | | -19.714 | 16.408 | 1.00 | 10.86 |
| ATOM | 6510 | ō | HIS | 968 | | -20.590 | 15.536 | 1.00 | 9.61 |
| ATOM | 6511 | N | THR | 969 | | -18.486 | 16.237 | | 10.09 |
| | 6512 | CA | THR | 969 | -2.135 | -18.099 | 15.001 | 1.00 | 8.73 |
| ATOM | | | | | | | | | |
| ATOM | 6513 | CB | THR | 969 | -2.773 | -16.698 | 15.148 | | 11.74 |
| MOTA | 6514 | | THR | 969 | | -16.774 | 16.066 | | 12.00 |
| MOTA | 6515 | CG2 | THR | 969 | | -16.182 | 13.791 | | 10.32 |
| MOTA | 6516 | С | THR | 969 | | -18.118 | 13.822 | | 10.38 |
| MOTA | 6517 | 0 | THR | 969 | -1.506 | -18.557 | 12.719 | 1.00 | 10.24 |
| MOTA | 6518 | N | ALA | 970 | 0.064 | -17.653 | 14.056 | 1.00 | 8.37 |
| ATOM | 6519 | CA | ALA | 970 | 1.076 | -17.624 | 13.001 | 1.0Ò | 9.33 |
| ATOM | 6520 | CB | ALA | 970 | 2.285 | -16.817 | 13.467 | 1.00 | 7.66 |
| ATOM | 6521 | С | ALA | 970 | | -19.046 | 12.608 | | 10.42 |
| ATOM | 6522 | ō | ALA | 970 | | -19.311 | 11.445 | | 10.11 |
| ATOM | 6523 | N | ALA | 971 | | -19.950 · | | 1.00 | 7.79 |
| | | | | | 1.437 | -21.345 | | | 8.64 |
| ATOM | 6524 | CA | ALA | 971 | | | 13.352 | 1.00 | |
| ATOM | 6525 | CB | ALA | 971 | 2.043 | -22.065 | 14.685 | | 10.14 |
| ATOM | 6526 | С | ALA | 971 | | -22.037 | 12.520 | 1.00 | 7.88 |
| ATOM | 6527 | 0 | ALA | 971 | 1.112 | -22.756 | 11.570 | | 10.59 |
| MOTA | 6528 | N | VAL | 972 | -0.447 | -21.816 | 12.892 | 1.00 | 9.57 |
| ATOM | 6529 | CA | VAL | 972 | -1.573 | -22.417 | 12.187 | 1.00 | 8.65 |
| ATOM | 6530 | CB | VAL | 972 | -2.901 | -22.072 | 12.910 | 1.00 | 8.10 |
| ATOM | 6531 | CG1 | VAL | 972 | -4.098 | -22.433 | 12.040 | 1.00 | 7.43 |
| ATOM | 6532 | | VAL | 972 | -2.978 | -22.839 | 14.231 | | 10.94 |
| ATOM | 6533 | C | VAL | 972 | -1.604 | -21.935 | 10.740 | | 10.50 |
| ATOM | 6534 | Ō | VAL | 972 | -1.813 | -22.725 | 9.815 | 1.00 | 8.95 |
| ATOM | 6535 | | ARG | 973 | | -20.641 | 10.548 | | 10.52 |
| | | | | | | | | | |
| ATOM | 6536 | CA | ARG | 973 | -1.359 | -20.052 | 9.206 | | 12.00 |
| ATOM | 6537 | CB | ARG | 973 | -1.179 | -18.526 | 9.291 | | 13.02 |
| MOTA | 6538 | CG | ARG | 973 | -1.127 | -17.808 | 7.926 | | 14.67 |
| MOTA | 6539 | CD | ARG | 973 | -2.343 | -18.128 | 7.055 | | 12.64 |
| ATOM | 6540 | NE | ARG | 973 | -3.543 | -17.405 | 7.457 | | 14.38 |
| ATOM | 6541 | CZ | ARG | 973 | -4.783 | -17.779 | 7.149 | 1.00 | 11.66 |
| ATOM | 6542 | NH1 | ARG | 973 | -4.993 | -18.879 | 6.440 | 1.00 | 15.11 |
| ATOM | 6543 | NH2 | ARG | 973 | -5.819 | -17.045 | 7.533 | 1.00 | 13.03 |
| ATOM | 6544 | С | ARG | 973 | | -20.666 | 8.349 | | 11.81 |
| ATOM | 6545 | ō | ARG | 973 | | -20.851 | 7.139 | | 13.18 |
| ATOM | 6546 | N | ARG | 974 | | -20.979 | 8.960 | 1.00 | 10.93 |
| ATOM | 6547 | CA | ARG | 974 | 1.971 | -21.585 | 8.194 | | 12.60 |
| | | | | | | -21.701 | 9.033 | | 10.96 |
| MOTA | 6548 | CB | ARG | 974 | | | | | |
| MOTA | 6549 | CG | ARG | 974 | | -20.370 | 9.472 | | 13.59 |
| MOTA | 6550 | CD | ARG | 974 | | -20.456 | 9.924 | | 15.74 |
| MOTA | 6551 | NE | ARG | 974 | | -19.147 | 10.394 | | 16.85 |
| ATOM · | 6552 | CZ | ARG | 974 | | -18.750 | 11.659 | | 18.61 |
| ATOM | 6553 | NH1 | ARG | 974 | 5.210 | -19.574 | 12.603 | 1.00 | 12.75 |
| ATOM | .6554 | NH2 | ARG | 974 | 5.984 | -17.502 | 11.972 | 1.00 | 19.12 |
| ATOM | 6555 | С | ARG . | 974 | 1.562 | -22.967 | 7.707 | 1.00 | 13.55 |
| ATOM | 6556 | 0 | ARG | 974 | 1.899 | -23.372 | 6.592 | 1.00 | 14.37 |
| ATOM | 6557 | N | GLY | 975 | 0.834 | -23.693 | 8.545 | | 13.23 |
| ATOM | 6558 | CA | GLY | 975 | | -25.026 | 8.164 | | 13.14 |
| ATOM | 6559 | C | GLY | 975 | -0.792 | -25.049 | 7.222 | | 12.25 |
| | | | | 975 | -0.957 | -26.002 | 6.462 | | 11.97 |
| ATOM | 6560 | 0 | GLY | | | -24.002 | | | |
| ATOM | 6561 | N | ALA | 976 | -1.617 | | 7.273 | | 11.12 |
| ATOM | 6562 | CA | ALA | 976 | | -23.896 | 6.441 | | 11.30 |
| ATOM | 6563 | CB | ALA | 976 | | -24.243 | 7.271 | | 10.07 |
| ATOM | 6564 | С | ALA | 976 | | -22.480 | 5.863 | | 13.51 |
| MOTA | 6565 | 0 | ALA | 976 | | -21.722 | 6.274 | | 12.15 |
| ATOM | 6566 | N | PRO | 977 | -2.118 | -22.114 | 4.889 | 1.00 | 14.78 |
| MOTA | 6567 | CD | PRO | 977 | -1.121 | -22.953 | 4.206 | 1.00 | 17.34 |
| MOTA | 6568 | CA | PRO | 977 | -2.179 | -20.773 | 4.288 | 1.00 | 15.20 |
| ATOM | 6569 | СВ | PRO | 977 | | -20.783 | 3.304 | 1.00 | 15.29 |
| ATOM | 6570 | CG | PRO | 977 | | -22.205 | 2.885 | | 20.17 |
| ATOM | 6571 | C | PRO | 977 | | -20.324 | 3.641 | | 15.15 |
| ATOM | 6572 | 0 | | 977 | | -19.121 | 3.486 | | 15.71 |
| | | | PRO | | | | 3.400 | | 15.08 |
| ATOM | 6573 | N | ASN | 978 | -4.348 | -21.270 | 3.4/3 | 1.00 | 10.00 |

| ATOM 6574 CA ASIN 978 -5.616 -20.924 2.631 1.00 16.97 ATOM 6575 CB ASIN 978 -4.692 -21.397 0.315 1.00 12.84 ATOM 6576 CG ASIN 978 -4.692 -21.397 0.315 1.00 24.37 ATOM 6577 OD1 ASIN 978 -4.692 -21.397 0.315 1.00 24.37 ATOM 6577 OD1 ASIN 978 -4.673 -20.322 -0.020 1.00 26.80 ATOM 6578 ND2 ASIN 978 -4.618 -22.423 -0.185 1.00 28.38 ATOM 6579 C ASIN 978 -4.018 -22.423 -0.185 1.00 28.38 ATOM 6580 N ASIN 978 -4.018 -22.423 -0.185 1.00 28.38 ATOM 6581 N CYS 979 -6.671 -21.37 3.497 1.00 15.81 ATOM 6581 N CYS 979 -7.828 -21.787 5.597 1.00 15.35 ATOM 6582 CA CYS 979 -7.828 -21.787 5.597 1.00 15.35 ATOM 6585 C CYS 979 -7.828 -21.787 5.597 1.00 15.35 ATOM 6585 C CYS 979 -7.828 -21.787 5.597 1.00 15.73 ATOM 6586 C CYS 979 -6.671 -21.757 8.193 1.00 17.53 ATOM 6586 N CYS 979 -7.829 -19.416 6.035 1.00 13.52 ATOM 6586 N CYS 979 -7.829 -19.416 6.035 1.00 13.52 ATOM 6586 N CYS 979 -7.829 -19.416 6.035 1.00 13.52 ATOM 6586 N CYS 979 -7.829 -19.416 6.035 1.00 13.69 ATOM 6580 C CYS 979 -7.829 -19.416 6.035 1.00 13.69 ATOM 6590 CC LEU 980 -1.19.41 -19.582 7.017 1.00 11.50 ATOM 6590 CC LEU 980 -1.19.41 -19.582 7.017 1.00 11.50 ATOM 6590 CC LEU 980 -1.19.41 -19.582 7.017 1.00 11.50 ATOM 6590 CC LEU 980 -1.19.41 -19.582 7.017 1.00 11.50 ATOM 6590 CC LEU 980 -1.19.41 -19.677 8.604 1.00 11.60 ATOM 6595 N LEU 981 -1.2.747 18.677 9.099 1.00 12.13 ATOM 6590 C CD LEU 980 -9.970 -19.627 8.604 1.00 11.62 ATOM 6595 N LEU 980 -9.970 -19.627 8.604 1.00 11.62 ATOM 6595 N LEU 981 -9.18 1.00 13.60 ATOM 6595 N LEU 981 -9.18 1.00 13.60 ATOM 6595 N LEU 981 -9.18 1.00 13.60 ATOM 6590 C CD LEU 980 -9.970 -19.627 8.604 1.00 11.00 11.00 11.00 ATOM 6590 C CD LEU 981 -9.19 1.00 1.30 ATOM 6590 C CD LEU 981 -9.19 1.00 1.30 ATOM 6590 C CD LEU 981 -9.19 1.00 ATOM 6590 C CD LEU 982 -9.19 1.00 ATOM 6 | | | | | | | | | |
|--|------|------|-----|-----|-----|---------|---------|--------|------------|
| ATOM 6576 CG ASN 978 -4.692 - 21.397 0.315 1.00 24.37 ATOM 6577 ODI ASN 978 -4.473 - 20.322 -0.020 1.00 26.80 ATOM 6578 NDZ ASN 978 -4.018 -22.423 -0.185 1.00 26.80 ATOM 6580 O ASN 978 -4.018 -22.423 -0.185 1.00 26.80 ATOM 6581 N CYS 979 -6.856 -21.37 3.475 1.00 15.81 ATOM 6581 N CYS 979 -7.828 -21.787 5.597 1.00 15.45 ATOM 6582 CA CYS 979 -7.828 -21.787 5.597 1.00 15.45 ATOM 6583 CB CYS 979 -7.828 -21.787 5.597 1.00 15.73 ATOM 6586 CYS 979 -7.427 -22.656 6.80 1.00 15.73 ATOM 6586 CYS 979 -7.829 -9.459 -0.945 6.096 1.00 15.73 ATOM 6586 CYS 979 -7.869 -19.416 6.035 1.00 15.73 ATOM 6586 CYS 979 -7.869 -19.416 6.035 1.00 15.73 ATOM 6587 N LEU 980 -10.396 -19.458 7.148 1.00 11.99 ATOM 6598 CB LEU 980 -10.396 -19.458 7.148 1.00 11.99 ATOM 6590 CG LEU 980 -12.747 -18.553 7.795 1.00 13.60 ATOM 6591 CD1 LEU 980 -12.747 -18.553 7.795 1.00 13.60 ATOM 6592 CD2 LEU 980 -12.439 -17.144 7.313 1.00 17.94 ATOM 6595 C LEU 980 -12.439 -17.44 7.313 1.00 17.94 ATOM 6595 C LEU 980 -10.336 -20.601 9.262 1.00 11.62 ATOM 6596 CA LEU 981 -9.970 -19.627 8.604 1.00 11.62 ATOM 6596 CA LEU 981 -9.167 -18.660 10.447 1.00 1.00 ATOM 6596 CA LEU 981 -9.187 -18.760 10.447 1.00 1.00 ATOM 6596 CA LEU 981 -9.474 -18.650 10.447 1.00 1.00 ATOM 6606 CG LEU 981 -9.474 -18.650 1.037 1.00 1.00 ATOM 6607 CDI LEU 982 -9.486 -19.394 1.595 1.00 1.00 1.00 ATOM 6607 CDI LEU 982 -9.486 -19.394 1.00 1.00 1.00 ATOM 6607 CDI LEU 982 -9.486 -19.348 1.00 1.00 1.00 ATOM 6607 COI LEU 98 | MOTA | 6574 | CA | ASN | 978 | -5.616 | -20.924 | 2.631 | 1.00 16.97 |
| ATOM 6576 CG ASN 978 -4.692 -21.397 0.315 1.00 24.37 ATOM 6577 ODI ASN 978 -4.473 -20.322 -0.022 1.00 24.80 26.80 ATOM 6579 C ASN 978 -4.018 -22.423 -0.185 1.00 28.38 ATOM 6579 C ASN 978 -4.018 -22.423 -0.185 1.00 28.38 ATOM 6579 C ASN 978 -4.018 -22.423 -0.185 1.00 28.38 ATOM 6581 N CYS 979 -6.685 -21.137 3.475 1.00 15.91 ATOM 6582 CA CYS 979 -7.828 -21.787 5.597 1.00 15.35 ATOM 6582 CA CYS 979 -7.828 -21.787 5.597 1.00 15.35 ATOM 6585 C CYS 979 -7.828 -21.787 5.597 1.00 15.35 ATOM 6586 CYS 979 -6.671 -21.757 8.193 1.00 17.53 ATOM 6586 C CYS 979 -6.617 -21.757 8.193 1.00 17.53 ATOM 6586 C CYS 979 -7.829 -19.416 6.035 1.00 13.52 ATOM 6586 C CYS 979 -7.829 -19.416 6.035 1.00 13.52 ATOM 6586 C CYS 979 -7.829 -19.416 6.035 1.00 13.52 ATOM 6586 C CYS 979 -7.829 -19.416 6.035 1.00 13.50 ATOM 6580 CB LEU 980 -10.336 -19.458 7.148 1.00 11.93 ATOM 6590 CB LEU 980 -10.336 -19.458 7.148 1.00 11.93 ATOM 6590 CB LEU 980 -12.747 -18.553 7.795 1.00 13.05 ATOM 6590 CB LEU 980 -12.747 -18.553 7.795 1.00 13.05 ATOM 6590 CB LEU 980 -12.249 -17.144 7.313 1.00 17.24 ATOM 6593 C LEU 980 -12.249 -18.871 7.628 1.00 13.60 ATOM 6590 CB LEU 980 -10.336 -20.601 9.262 1.00 13.60 ATOM 6590 CB LEU 980 -10.336 -20.601 9.262 1.00 13.60 ATOM 6590 CB LEU 980 -10.336 -20.601 9.262 1.00 13.60 ATOM 6590 CB LEU 980 -10.336 -20.601 9.262 1.00 13.60 ATOM 6590 CB LEU 980 -10.336 -20.601 9.262 1.00 13.60 ATOM 6590 CB LEU 980 -10.336 -20.601 9.262 1.00 13.60 ATOM 6590 CB LEU 980 -10.336 -20.601 9.262 1.00 13.60 ATOM 6590 CB LEU 981 -6.642 -18.797 1.00 11.01 1.01 1.01 1.01 1.01 1.01 1. | ATOM | 6575 | CB | ASN | 978 | -5.770 | -21.725 | 1.330 | 1.00 21.84 |
| ATOM 6577 DDJ ASN 978 -4.473 -20.232 -0.020 1.00 26.89 ATOM 6579 C ASN 978 -6.856 -21.137 3.497 1.00 15.85 ATOM 6580 C ASN 978 -6.856 -21.137 3.497 1.00 15.95 ATOM 6580 C ASN 978 -6.671 -21.541 4.745 1.00 15.45 ATOM 6581 N CYS 979 -6.671 -21.541 4.745 1.00 15.45 ATOM 6582 CA CYS 979 -7.827 -12.787 5.579 1.00 15.35 ATOM 6583 CB CYS 979 -7.427 -22.656 6.803 1.00 15.73 ATOM 6585 C CYS 979 -7.427 -22.656 6.803 1.00 15.75 ATOM 6586 C CYS 979 -7.427 -22.656 6.803 1.00 15.76 ATOM 6586 C CYS 979 -7.427 -22.656 6.803 1.00 15.76 ATOM 6586 C CYS 979 -8.469 -20.495 6.096 1.00 13.56 ATOM 6586 C CYS 979 -8.469 -20.495 6.096 1.00 13.56 ATOM 6586 C CYS 979 -7.827 -1.05 4.00 4.00 15.76 ATOM 6587 N LEU 980 -9.709 -20.603 6.559 1.00 15.76 ATOM 6587 N LEU 980 -9.709 -20.603 6.559 1.00 15.96 ATOM 6589 CB LEU 980 -11.914 -19.582 7.017 1.00 13.15 ATOM 6590 CG LEU 980 -11.914 -19.582 7.017 1.00 13.09 ATOM 6590 CG LEU 980 -12.439 -17.144 7.313 1.00 17.24 ATOM 6590 CD LEU 980 -9.970 -19.627 8.604 1.00 11.63 ATOM 6590 CD LEU 980 -9.970 -19.627 8.604 1.00 11.63 ATOM 6590 CD LEU 980 -9.970 -19.627 8.604 1.00 11.63 ATOM 6590 CD LEU 980 -9.970 -19.627 8.604 1.00 11.63 ATOM 6590 CD LEU 980 -9.970 -19.627 8.604 1.00 11.63 ATOM 6590 CD LEU 980 -9.970 -19.627 8.604 1.00 11.63 ATOM 6590 CD LEU 981 -9.187 -18.677 9.099 1.00 12.13 ATOM 6590 CD LEU 981 -9.187 -18.677 9.099 1.00 12.13 ATOM 6590 CD LEU 981 -9.187 -18.677 9.099 1.00 12.13 ATOM 6590 CD LEU 981 -9.187 -18.679 10.387 1.00 12.12 ATOM 6600 CD LEU 981 -9.197 -16.647 1.1977 12.747 1.00 15.77 ATOM 6600 CD LEU 981 -9.197 -16.647 1.1977 12.747 1.00 15.75 ATOM 6600 CD LEU 981 -9.197 -16.647 1.1977 12.747 1.00 15.74 ATOM 6600 CD LEU 981 -9.197 -16.647 1.1977 12.747 1.00 12.12 ATOM 6601 C LEU 981 -9.197 -16.647 1.1977 12.747 1.00 12.74 ATOM 6601 C LEU 981 -9.909 -19.797 -19.688 1.00 11.00 11.18 ATOM 6601 C LEU 981 -9.197 -16.647 1.1977 12.747 1.00 12.74 ATOM 6601 C ADOM 6607 CD LEU 982 -19.909 -19.707 -19.688 1.00 11.00 11.18 ATOM 6600 C C LEU 982 -19.909 -19.707 -19.689 11.00 11.19 1.00 11.19 ATOM | ATOM | 6576 | CG | ASN | 978 | -4.692 | -21.397 | 0.315 | 1.00 24.37 |
| ATOM 6578 NDZ ASN 978 -4.018 -22.423 -0.185 1.00 28.38 ATOM 6579 C ASN 978 -6.856 -21.317 3.475 1.00 15.81 ATOM 6580 N CYS 979 -6.856 -21.317 3.475 1.00 15.93 ATOM 6581 N CYS 979 -7.828 -21.787 5.597 1.00 15.93 ATOM 6582 CA CYS 979 -7.828 -21.787 5.597 1.00 15.93 ATOM 6582 CA CYS 979 -7.828 -21.787 5.597 1.00 15.93 ATOM 6586 C CYS 979 -6.671 -21.757 8.193 1.00 17.53 ATOM 6586 C CYS 979 -6.671 -21.757 8.193 1.00 17.53 ATOM 6586 C CYS 979 -6.671 -21.757 8.193 1.00 17.53 ATOM 6586 C CYS 979 -7.829 -19.416 6.035 1.00 15.73 ATOM 6586 C CYS 979 -7.829 -19.416 6.035 1.00 15.73 ATOM 6586 C CYS 979 -7.829 -19.416 6.035 1.00 15.73 ATOM 6586 C CYS 979 -7.829 -19.416 6.035 1.00 15.73 ATOM 6587 N LEU 980 -9.709 -20.63 6.559 1.00 15.60 ATOM 6588 CA LEU 980 -10.396 -19.588 7.148 1.00 11.93 ATOM 6590 CB LEU 980 -11.914 -19.582 7.017 1.00 13.50 ATOM 6590 CB LEU 980 -11.914 -19.582 7.017 1.00 13.05 ATOM 6590 CB LEU 980 -12.747 -18.553 7.795 1.00 13.60 ATOM 6595 C DLEU 980 -12.249 -11.94 7.628 1.00 13.60 ATOM 6595 C LEU 980 -9.970 -19.627 8.664 1.00 11.80 ATOM 6595 N LEU 980 -9.970 -19.627 8.664 1.00 11.80 ATOM 6595 N LEU 981 -9.970 -19.627 8.664 1.00 12.13 ATOM 6596 CA LEU 981 -7.132 -18.760 10.447 1.00 15.93 ATOM 6596 CA LEU 981 -7.132 -18.760 10.447 1.00 15.93 ATOM 6696 C C LEU 981 -6.195 -18.853 11.539 1.00 12.10 ATOM 6600 CD2 LEU 981 -6.195 -18.853 11.539 1.00 12.10 ATOM 6600 CD2 LEU 981 -6.195 -18.853 11.539 1.00 12.10 ATOM 6600 CD2 LEU 981 -6.195 -18.853 11.539 1.00 12.10 ATOM 6600 CD2 LEU 981 -9.197 -16.604 11.321 1.00 11.03 ATOM 6606 C C LEU 981 -9.197 -15.604 11.321 1.00 11.03 ATOM 6606 C C LEU 981 -9.197 -15.604 11.321 1.00 11.03 ATOM 6606 C C LEU 981 -9.197 -15.604 11.321 1.00 11.03 ATOM 6606 C C LEU 982 -1.0604 -1.07.532 14.951 1.00 12.07 ATOM 6606 C C LEU 982 -9.198 -18.521 14.951 1.00 11.03 ATOM 6616 C LEU 982 -9.198 -18.521 1.00 11.00 11.03 ATOM 6616 C C LEU 982 -9.994 -18.521 1.00 11.03 1.83 ATOM 6606 C C LEU 982 -9.994 -18.521 1.00 11.00 11.03 ATOM 6608 C C LEU 985 -1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.0 | | | OD1 | ASN | 978 | -4.473 | -20.232 | -0.020 | 1.00 26.80 |
| ATOM 6579 C ASN 978 -6.856 -21.137 3.497 1.00 15.81 ATOM 6580 O ASN 978 -7.978 -20.99 3.06 1.00 16.34 ATOM 6581 N CYS 979 -6.671 -21.541 4.745 1.00 15.45 ATOM 6582 CA CYS 979 -7.828 -21.787 5.797 1.00 15.35 ATOM 6583 CB CYS 979 -7.427 -22.556 6.803 1.00 15.73 ATOM 6585 C CYS 979 -7.427 -22.556 6.803 1.00 15.73 ATOM 6585 C CYS 979 -8.469 -20.495 6.096 1.00 15.56 ATOM 6585 C CYS 979 -8.469 -20.495 6.096 1.00 15.57 ATOM 6586 O CYS 979 -8.469 -20.495 6.096 1.00 15.57 ATOM 6586 O CYS 979 -8.469 -20.495 6.096 1.00 15.57 ATOM 6586 O CYS 979 -7.889 -19.416 6.053 1.00 15.76 ATOM 6587 N LEU 980 -9.709 -20.603 6.559 1.00 13.59 ATOM 6580 CG LEU 980 -10.396 -19.458 7.148 1.00 11.99 ATOM 6589 CB LEU 980 -11.914 -19.582 7.017 1.00 13.19 ATOM 6590 CG LEU 980 -12.747 -18.553 7.795 1.00 13.50 ATOM 6590 CG LEU 980 -12.747 -18.553 7.795 1.00 13.50 ATOM 6590 CG LEU 980 -9.970 -19.627 8.604 1.00 11.29 ATOM 6590 CG LEU 980 -9.970 -19.627 8.604 1.00 11.63 ATOM 6595 N LEU 980 -9.970 -19.627 8.604 1.00 11.63 ATOM 6595 N LEU 980 -9.970 -19.627 8.604 1.00 11.63 ATOM 6595 N LEU 980 -9.970 -19.627 8.604 1.00 11.63 ATOM 6595 N LEU 981 -9.187 -18.677 9.099 1.00 12.18 ATOM 6595 N LEU 981 -9.187 -18.677 9.099 1.00 12.18 ATOM 6590 CC LEU 981 -9.18 ATOM 6590 CC LEU 981 -9.19 -1.867 ATOM 6590 CC LEU 982 -1.19 ATOM 6590 CC LEU 985 -1.19 ATOM 6590 CC LEU 985 | | | | | 978 | | -22.423 | | |
| ATOM 6580 O ASN 978 | | | | | | | | | |
| ATOM 6581 N CYS 979 | | | | | | | | | |
| ATOM 6582 CB CYS 979 -7.427 -22.656 6.093 1.00 15.73 ATOM 6588 CB CYS 979 -6.617 -21.757 8.193 1.00 15.73 ATOM 6585 C CYS 979 -6.617 -21.757 8.193 1.00 17.53 ATOM 6585 C CYS 979 -8.469 -19.416 6.035 1.00 13.52 ATOM 6586 C CYS 979 -7.827 -22.656 6.096 1.00 13.52 ATOM 6587 N LEU 980 -9.709 -20.633 6.559 1.00 13.62 ATOM 6589 CB LEU 980 -10.336 -19.458 7.148 1.00 13.95 ATOM 6590 CB LEU 980 -11.914 -19.582 7.017 1.00 13.55 ATOM 6591 CB LEU 980 -12.439 -17.144 7.017 1.00 13.15 ATOM 6591 CD LEU 980 -12.439 -17.144 7.313 1.00 17.24 ATOM 6592 CD LEU 980 -12.439 -17.144 7.313 1.00 17.24 ATOM 6593 C LEU 980 -1.362 -19.458 7.795 1.00 13.05 ATOM 6594 C LEU 980 -1.2439 -17.144 7.313 1.00 17.24 ATOM 6595 N LEU 980 -1.362 -22.660 9.262 1.00 11.62 ATOM 6595 N LEU 980 -1.036 -22.660 9.262 1.00 11.62 ATOM 6595 N LEU 981 -9.167 -18.677 9.099 1.00 12.13 ATOM 6596 CA LEU 981 -9.167 -18.677 9.099 1.00 12.13 ATOM 6596 CA LEU 981 -5.167 -18.670 1.0347 1.00 19.95 ATOM 6597 CB LEU 981 -5.167 -18.670 1.0347 1.00 10.99 ATOM 6598 CG LEU 981 -6.195 -18.853 11.539 1.00 12.12 ATOM 6600 CD LEU 981 -6.195 -18.853 11.539 1.00 12.12 ATOM 6600 CD LEU 981 -6.472 -17.977 12.747 1.00 15.27 ATOM 6600 CD LEU 981 -6.472 -17.977 12.474 1.00 15.27 ATOM 6600 CD LEU 981 -9.197 -16.604 11.321 1.00 1.52.7 ATOM 6600 CD LEU 982 -19.984 -18.394 12.445 1.00 13.63 ATOM 6606 C LEU 982 -19.982 -19.984 -18.394 12.445 1.00 13.63 ATOM 6606 C LEU 982 -19.687 -18.683 11.75 1.00 13.63 ATOM 6607 CD LEU 982 -19.687 -18.680 11.75 1.00 13.63 ATOM 6608 CD LEU 982 -19.987 -18.680 11.715 1.00 13.63 ATOM 6608 CD LEU 982 -19.982 -19.1840 11.715 1.00 13.63 ATOM 6607 CD LEU 982 -19.687 -18.680 11.715 1.00 13.63 ATOM 6608 CD LEU 982 -19.687 -18.680 11.715 1.00 13.63 ATOM 6608 CD LEU 982 -19.687 -18.680 11.715 1.00 13.63 ATOM 6608 CD LEU 982 -9.197 -18.680 11.715 1.00 13.63 ATOM 6608 CD LEU 982 -19.687 -18.681 11.715 1.00 13.63 ATOM 6608 CD LEU 982 -19.682 -19.683 11.693 1.00 10.13 ATOM 6608 CD LEU 982 -19.682 -19.683 11.00 10.10 1.00 11.20 1.00 11.20 1.00 11.20 1.00 1.0 | | | | | | | | | |
| ATOM 6583 CB CYS 979 | | | | | | | | | |
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| ATOM 6585 C CYS 979 - 8.469 -20.495 6.996 1.00 13.526 ATOM 6587 N LEU 980 -9.709 -20.603 6.559 1.00 15.76 ATOM 6588 CA LEU 980 -9.709 -20.603 6.559 1.00 13.00 ATOM 6589 CB LEU 980 -10.396 -19.458 7.097 1.00 13.00 ATOM 6590 CG LEU 980 -12.747 -18.553 7.097 1.00 13.00 ATOM 6591 CD1 LEU 980 -12.747 -18.553 7.795 1.00 13.00 ATOM 6593 C LEU 980 -12.747 -18.553 7.795 1.00 13.00 ATOM 6593 C LEU 980 -12.747 -18.553 7.955 1.00 13.00 ATOM 6593 C LEU 980 -12.747 -18.553 7.955 1.00 13.00 ATOM 6594 O LEU 980 -14.229 -18.871 7.628 1.00 13.00 ATOM 6595 N LEU 980 -10.336 -20.601 9.262 1.00 11.62 ATOM 6596 CA LEU 980 -10.336 -20.601 9.262 1.00 11.62 ATOM 6597 CB LEU 981 -8.647 -18.677 0.999 1.00 12.13 ATOM 6598 CC LEU 981 -8.647 -18.676 10.447 1.00 9.55 ATOM 6599 CD LEU 981 -6.195 -18.893 11.539 1.00 12.13 ATOM 6590 CD LEU 981 -6.4741 -18.706 11.090 1.00 12.07 ATOM 6600 C LEU 981 -6.472 -17.977 12.747 1.00 12.07 ATOM 6601 C LEU 981 -9.901 -17.827 11.448 1.00 10.37 ATOM 6606 CG LEU 981 -9.917 -16.604 11.321 1.00 1.03 ATOM 6606 CG LEU 982 -11.948 18.1341 13.951 1.00 10.37 ATOM 6606 CG LEU 982 -11.948 18.1341 13.951 1.00 10.37 ATOM 6606 CG LEU 982 -11.948 18.1341 13.951 1.00 10.12.12 ATOM 6607 CD LEU 982 -11.948 18.1341 13.951 1.00 10.12.12 ATOM 6608 CD LEU 982 -11.948 18.140 13.395 1.00 12.12 ATOM 6606 CG LEU 982 -11.948 18.140 13.295 1.00 13.85 ATOM 6607 CD LEU 982 -11.948 18.140 13.295 1.00 13.85 ATOM 6608 CD LEU 982 -11.948 18.140 13.295 1.00 10.13.85 ATOM 6608 CD LEU 982 -19.945 -18.834 12.595 1.00 13.85 ATOM 6608 CD LEU 982 -19.945 -18.834 12.595 1.00 13.85 ATOM 6608 CD LEU 982 -10.604 -17.554 13.495 1.00 10.13.85 ATOM 6608 CD LEU 982 -10.604 -17.554 13.495 1.00 10.13.85 ATOM 6608 CD LEU 982 -10.604 -17.554 13.695 1.00 13.85 ATOM 6608 CD LEU 982 -10.604 -17.554 13.695 1.00 13.85 ATOM 6608 CD LEU 982 -10.604 -17.554 13.695 1.00 13.85 ATOM 6608 CD LEU 982 -10.604 -17.554 13.695 1.00 13.85 ATOM 6608 CD LEU 982 -10.604 -17.554 13.695 1.00 13.85 ATOM 6608 CD LEU 982 -10.604 -17.554 13.695 1.00 13.85 ATOM 6608 CD LEU 982 -10.604 - | MOTA | 6583 | CB | CYS | | | | | |
| ATOM 6586 O CVS 979 -7.869 -19.416 6.035 1.00 15.76 1.00 13.60 ATOM 6588 C Cale LEU 980 -9.709 -20.603 6.559 1.00 13.60 ATOM 6589 CB CB LEU 980 -11.914 -19.582 7.017 1.00 13.10 13.15 ATOM 6590 CB CB LEU 980 -12.247 -18.553 7.795 1.00 13.09 13.09 ATOM 6592 CD CD LEU 980 -12.439 -17.144 7.313 1.00 17.24 10.01 13.60 ATOM 6593 CD CEU 980 -19.30 -19.627 8.604 1.00 11.60 13.09 ATOM 6595 N LEU 981 -9.187 -18.677 9.099 1.00 12.13 ATOM 6597 CB EU 981 -9.187 -18.677 9.099 1.00 12.13 ATOM 6599 CD LEU 981 -6.132 18.853 1.539 1.00 12.13 ATOM 6601 C LEU 981 -6.172 18.607 9.099 1.00 12.13 | MOTA | 6584 | SG | CYS | 979 | -6.617 | -21.757 | 8.193 | 1.00 17.53 |
| ATOM 6587 N LEU 980 | ATOM | 6585 | С | CYS | 979 | -8.469 | -20.495 | 6.096 | 1.00 13.52 |
| ATOM 6588 CA LEU 980 -9.709 -20.603 6.559 1.00 13.60 ATOM 6588 CA LEU 980 -10.396 -19.458 7.148 1.00 11.99 ATOM 6590 CG LEU 980 -11.914 -19.582 7.017 1.00 13.15 ATOM 6591 CD1 LEU 980 -12.747 -18.553 7.795 1.00 13.09 ATOM 6592 CD2 LEU 980 -12.439 -17.144 7.313 1.00 17.24 ATOM 6593 C LEU 980 -12.439 -17.144 7.313 1.00 17.24 ATOM 6593 C LEU 980 -9.970 -19.627 8.604 1.00 11.62 ATOM 6595 C LEU 980 -9.970 -19.627 8.604 1.00 11.63 ATOM 6595 N LEU 981 -9.187 -18.677 9.099 1.00 12.13 ATOM 6596 CA LEU 981 -9.187 -18.677 9.099 1.00 12.13 ATOM 6597 CB LEU 981 -6.195 -18.853 11.539 1.00 10.95 ATOM 6598 CG LEU 981 -6.195 -18.853 11.539 1.00 12.12 ATOM 6600 CD2 LEU 981 -6.474 1.87.60 11.090 1.00 12.71 ATOM 6601 C LEU 981 -6.474 1.87.60 11.090 1.00 12.71 ATOM 6601 C LEU 981 -9.910 -17.827 11.448 1.00 10.37 ATOM 6602 O LEU 981 -9.910 -17.827 11.448 1.00 10.37 ATOM 6603 N LEU 981 -9.910 -17.827 11.448 1.00 10.37 ATOM 6604 CA LEU 981 -9.910 -17.864 13.485 1.00 10.87 ATOM 6606 CB LEU 982 -11.948 -18.140 13.951 1.00 11.18 ATOM 6606 CB LEU 982 -11.948 -18.140 13.951 1.00 12.12 ATOM 6606 CB LEU 982 -11.948 -18.140 13.951 1.00 12.42 ATOM 6606 CB LEU 982 -11.948 -18.140 13.795 1.00 13.85 ATOM 6607 CD1 LEU 982 -12.997 -18.480 11.715 1.00 13.85 ATOM 6607 CD1 LEU 982 -12.997 -18.480 11.715 1.00 12.49 ATOM 6610 N LEU 982 -13.182 -17.866 13.095 1.00 12.49 ATOM 6611 N ALA 983 -9.455 -15.676 16.00 15.364 1.00 11.23 ATOM 6612 CA ALA 983 -9.959 -16.8521 14.951 1.00 12.49 ATOM 6616 N ASP 984 -10.136 -17.532 14.675 1.00 12.49 ATOM 6617 CA ASP 984 -10.136 -17.542 16.237 1.00 14.80 ATOM 6618 CB ASP 984 -10.106 -18.77 18.829 1.00 10.62 ATOM 6618 CB ASP 984 -10.106 -18.77 18.829 1.00 10.62 ATOM 6618 CB LEU 985 -10.043 -18.146 11.00 11.03 ATOM 6610 N LEU 985 -10.043 -18.146 11.00 11.00 1.00 ATOM 6611 CB ALA 983 -9.455 -15.676 21.60 11.00 11.00 1.00 ATOM 6612 CB LEU 985 -10.043 -11.810 11.00 11.00 1.00 ATOM 6613 CB LEU 985 -10.043 -11.810 11.00 11.00 1.00 ATOM 6614 CB LEU 985 -10.043 -11.810 11.00 11.00 1.00 ATOM 6615 CB LEU 985 -10.043 -11.295 21.763 | ATOM | 6586 | 0 | CYS | 979 | -7.869 | -19.416 | 6.035 | 1.00 15.76 |
| ATOM 6588 CA LEU 980 -10.396 -19.458 7.148 1.00 11.99 ATOM 6599 CB LEU 980 -11.914 -19.582 7.017 1.00 13.159 ATOM 6591 CDI LEU 980 -12.439 -17.144 7.313 1.00 17.244 ATOM 6592 CD2 LEU 980 -12.439 -17.144 7.313 1.00 17.244 ATOM 6593 C LEU 980 -12.439 -17.144 7.313 1.00 17.244 ATOM 6595 N LEU 980 -10.336 -20.601 9.262 1.00 13.80 ATOM 6595 N LEU 980 -10.336 -20.601 9.262 1.00 13.80 ATOM 6595 N LEU 981 -9.187 -18.677 9.099 1.00 12.13 ATOM 6596 CA LEU 981 -8.647 18.760 10.447 1.00 9.55 ATOM 6597 CB LEU 981 -6.195 -18.853 11.539 1.00 12.03 ATOM 6598 CG LEU 981 -6.195 -18.853 11.539 1.00 12.07 ATOM 6600 CD2 LEU 981 -6.472 -17.977 12.747 1.00 15.27 ATOM 6601 C LEU 981 -9.301 -17.827 11.448 1.00 10.37 ATOM 6602 C LEU 981 -9.301 -17.827 11.448 1.00 10.37 ATOM 6606 CD LEU 981 -9.301 -17.827 11.448 1.00 10.37 ATOM 6606 C LEU 982 -10.604 -17.564 11.321 1.00 11.83 ATOM 6605 CB LEU 982 -10.604 -17.564 13.485 1.00 18.37 ATOM 6606 CD LEU 982 -10.604 -17.564 13.485 1.00 18.37 ATOM 6607 CD1 LEU 982 -10.604 -17.564 13.485 1.00 18.37 ATOM 6608 CD2 LEU 982 -11.948 -18.140 13.951 1.00 12.12 ATOM 6608 CD2 LEU 982 -11.948 -18.140 13.951 1.00 12.12 ATOM 6607 CD1 LEU 982 -13.182 -17.868 13.095 1.00 13.85 ATOM 6608 CD2 LEU 982 -13.182 -17.868 13.095 1.00 13.85 ATOM 6608 CD2 LEU 982 -13.182 -17.868 13.095 1.00 13.85 ATOM 6608 CD2 LEU 982 -13.182 -17.868 13.095 1.00 13.85 ATOM 6608 CD2 LEU 982 -13.182 -17.868 13.095 1.00 13.85 ATOM 6608 CD2 LEU 982 -13.182 -17.868 13.095 1.00 13.85 ATOM 6608 CD2 LEU 982 -14.414 -18.442 13.792 1.00 14.38 ATOM 6608 CD2 LEU 982 -19.659 -17.532 14.675 1.00 12.49 ATOM 6608 CD2 LEU 982 -19.659 -17.532 14.675 1.00 12.49 ATOM 6608 CD2 LEU 982 -19.659 -17.532 14.675 1.00 13.85 ATOM 6608 CD2 LEU 982 -19.659 -17.532 14.675 1.00 13.85 ATOM 6608 CD2 LEU 985 -10.537 -10.50 2.479 1.00 14.08 ATOM 6608 CD2 LEU 985 -10.537 -10.50 2.479 1.00 14.08 ATOM 6608 CD2 LEU 985 -10.537 -10.50 2.479 1.00 14.09 ATOM 6608 CD2 LEU 985 -10.537 -10.50 2.479 1.00 14.09 ATOM 6608 CD2 LEU 985 -10.537 -10.50 2.479 1.00 14.09 ATOM 6608 CD2 LEU 98 | | 6587 | N | LEU | 980 | -9.709 | -20.603 | 6.559 | 1.00 13.60 |
| ATOM 6589 CB LEU 980 | | | | | | -10.396 | -19.458 | | 1.00 11.99 |
| ATOM 6590 CG LEU 980 -12.439 -17.144 7.313 1.00 17.24 ATOM 6591 CDI LEU 980 -29.970 -19.627 8.604 1.00 13.80 ATOM 6593 C LEU 980 -10.336 -20.601 9.262 1.00 13.80 ATOM 6595 N LEU 981 -9.970 -19.627 8.604 1.00 11.62 ATOM 6595 N LEU 981 -9.187 -18.677 9.099 1.00 12.13 ATOM 6596 CA LEU 981 -8.647 -18.760 10.447 1.00 9.55 ATOM 6597 CB LEU 981 -8.647 -18.760 10.447 1.00 9.55 ATOM 6598 CG LEU 981 -6.195 -18.853 11.539 1.00 12.07 ATOM 6599 CDI LEU 981 -6.195 -18.853 11.539 1.00 12.07 ATOM 6600 CD2 LEU 981 -6.472 -17.977 12.747 1.00 15.27 ATOM 6601 C LEU 981 -9.301 -17.827 12.747 1.00 15.27 ATOM 6602 C LEU 981 -9.301 -17.827 12.747 1.00 15.27 ATOM 6603 N LEU 982 -9.984 -18.394 12.445 1.00 10.37 ATOM 6606 CG LEU 982 -10.604 -17.564 13.485 1.00 10.87 ATOM 6606 CG LEU 982 -11.948 -18.140 13.951 1.00 12.13 ATOM 6607 CD1 LEU 982 -10.604 -17.564 13.495 10.00 13.63 ATOM 6607 CD1 LEU 982 -11.948 -18.140 13.951 1.00 12.83 ATOM 6608 CD2 LEU 982 -11.948 -18.140 13.951 1.00 12.83 ATOM 6608 CD2 LEU 982 -12.997 -18.480 13.095 1.00 13.63 ATOM 6607 CD1 LEU 982 -12.997 -18.480 13.095 1.00 13.63 ATOM 6610 O LEU 982 -9.659 -17.532 14.675 1.00 12.63 ATOM 6611 N ALA 983 -9.579 -16.400 15.364 10.00 13.83 ATOM 6610 N ASP 984 -10.108 -15.544 13.495 1.00 12.63 ATOM 6611 N ALA 983 -9.579 -16.400 15.364 10.00 11.28 ATOM 6612 CA ALA 983 -9.455 -15.676 17.682 1.00 13.63 ATOM 6616 N ASP 984 -10.108 -16.871 1.495 1.00 12.63 ATOM 6617 CA ASP 984 -10.108 -16.871 1.495 1.00 12.83 ATOM 6610 N ASP 984 -10.108 -16.871 1.00 12.83 ATOM 6617 CA ASP 984 -10.108 -16.871 1.148 1.00 1.00 1.78 ATOM 6620 CD LEU 985 -9.655 -17.532 1.4.675 1.00 12.63 ATOM 6617 CA ASP 984 -10.108 -16.871 1.148 1.00 1.00 1.78 ATOM 6620 CD ASP 984 -10.108 -16.871 1.00 12.83 ATOM 6617 CA ASP 984 -10.108 -16.871 1.00 12.83 ATOM 6618 CB SAP 984 -10.108 -16.871 1.00 12.83 ATOM 6619 CR SP 985 -9.529 -17.532 20.00 1.00 1.00 1.79 ATOM 6620 CD LEU 985 -9.659 -17.532 20.00 1.00 1.00 1.79 ATOM 6621 CD ASP 984 -10.108 -10.97 1.10 1.00 1.00 1.79 ATOM 6622 CR SP 984 -10.108 -10.97 1.10 1.00 1.00 1.7 | | | | | | | | | |
| ATOM 6591 CD1 LEU 980 -14.229 -18.871 7.628 1.00 13.80 ATOM 6592 CD2 LEU 980 -9.970 -19.627 8.604 1.00 11.62 ATOM 6595 N LEU 980 -9.970 -19.627 8.604 1.00 11.62 ATOM 6595 N LEU 981 -0.187 -18.677 9.099 1.00 12.13 ATOM 6596 CA LEU 981 -9.187 -18.677 9.099 1.00 12.13 ATOM 6597 CB LEU 981 -6.195 -18.853 11.539 1.00 12.23 ATOM 6598 CG LEU 981 -6.195 -18.853 11.539 1.00 12.23 ATOM 6500 CD2 LEU 981 -6.474 1.8.706 11.099 1.00 12.13 ATOM 6601 CD2 LEU 981 -6.474 1.8.706 11.099 1.00 12.13 ATOM 6601 C LEU 981 -9.197 -16.604 11.321 1.00 11.52 ATOM 6602 O LEU 981 -9.197 -16.604 11.321 1.00 11.18 ATOM 6603 N LEU 982 -9.984 +18.394 12.445 1.00 10.37 ATOM 6606 CG LEU 982 -11.948 -18.140 13.951 1.00 12.27 ATOM 6606 CG LEU 982 -11.948 -18.140 13.951 1.00 12.37 ATOM 6606 CG LEU 982 -11.948 -18.140 13.951 1.00 12.37 ATOM 6607 CD LEU 982 -11.948 -18.140 13.951 1.00 12.87 ATOM 6608 CD2 LEU 982 -11.948 -18.140 13.951 1.00 12.87 ATOM 6608 CD2 LEU 982 -11.948 -18.140 13.951 1.00 12.87 ATOM 6608 CD2 LEU 982 -11.948 -18.140 13.951 1.00 12.87 ATOM 6608 CD2 LEU 982 -11.948 -18.140 13.951 1.00 12.49 ATOM 6608 CD2 LEU 982 -12.997 -18.480 13.951 1.00 12.49 ATOM 6610 O LEU 982 -9.659 -17.532 14.675 1.00 12.49 ATOM 6610 O LEU 982 -9.659 -17.532 14.675 1.00 12.49 ATOM 6611 N ALA 983 -9.455 -15.676 16.533 1.00 11.23 ATOM 6612 CA ALA 983 -9.740 -15.542 16.237 1.00 14.38 ATOM 6613 CB ALA 983 -9.455 -15.676 16.00 15.364 1.00 11.00 ATOM 6610 N ASP 984 -10.108 -16.871 1.145 1.00 1.62 ATOM 6610 N ASP 984 -10.108 -16.871 2.149 1.00 1.00 1.00 ATOM 6610 N ASP 984 -10.108 -16.871 2.149 1.00 10.62 ATOM 6610 N ASP 984 -10.108 -16.871 2.149 1.00 10.63 ATOM 6610 N ASP 984 -10.108 -16.871 2.149 1.00 10.63 ATOM 6620 CD1 ASP 984 -10.108 -16.871 2.149 1.00 10.63 ATOM 6630 N EU 982 -13.481 -9.300 -14.291 2.149 1.00 10.63 ATOM 6630 N EU 982 -13.481 -9.300 -14.291 2.149 1.00 10.63 ATOM 6630 N EU 985 -10.991 -10.510 2.049 1.00 10.63 ATOM 6630 N EU 985 -10.991 -10.510 2.049 1.00 10.63 ATOM 6631 CD RUB 985 -10.091 -10.510 2.049 1.00 10.63 ATOM 6630 N EU 985 -10.991 -10. | | | | | | | | | |
| ATOM 6593 CD LEU 980 -14.229 -18.871 7.628 1.00 13.80 ATOM 6595 0 LEU 980 -9.970 -19.627 8.604 1.00 11.81 ATOM 6596 CA LEU 981 -9.187 -18.677 9.099 1.00 12.13 ATOM 6596 CA LEU 981 -8.647 -18.760 10.447 1.00 1.99 ATOM 6597 CB LEU 981 -6.195 -18.853 11.539 1.00 12.13 ATOM 6598 CG LEU 981 -6.195 -18.853 11.539 1.00 12.07 ATOM 6599 CD1 LEU 981 -6.472 -17.977 12.747 1.00 15.27 ATOM 6600 CD2 LEU 981 -6.472 -17.977 12.747 1.00 15.27 ATOM 6601 C LEU 981 -9.301 -17.827 11.448 1.00 10.37 ATOM 6602 C LEU 981 -9.981 -9.981 1.00 12.07 ATOM 6603 N LEU 982 -9.984 -18.394 12.445 1.00 10.37 ATOM 6606 CD2 LEU 981 -9.197 -16.604 11.321 1.00 11.81 ATOM 6606 CD2 LEU 982 -10.604 -17.564 13.485 1.00 10.37 ATOM 6606 CD2 LEU 982 -10.604 -17.564 13.495 1.00 12.12 ATOM 6606 CD2 LEU 982 -10.604 -17.564 13.495 1.00 12.12 ATOM 6607 CD1 LEU 982 -11.948 -18.140 13.951 1.00 12.12 ATOM 6608 CD2 LEU 982 -11.948 -18.140 13.951 1.00 12.12 ATOM 6608 CD2 LEU 982 -11.948 -18.140 13.951 1.00 12.12 ATOM 6609 C LEU 982 -12.997 18.801 11.715 1.00 13.63 ATOM 6610 N LEU 982 -12.997 18.801 11.715 1.00 13.63 ATOM 6610 N LAW 983 -9.579 16.400 15.364 1.00 11.28 ATOM 6610 N LAW 983 -9.579 16.400 15.364 1.00 11.28 ATOM 6610 N LAW 983 -9.579 16.600 15.364 1.00 11.28 ATOM 6610 N LAW 983 -9.579 16.600 15.364 1.00 11.28 ATOM 6611 N ALA 983 -9.455 -15.676 17.682 1.00 12.63 ATOM 6616 N ASP 984 -10.106 11.5825 20.266 1.00 11.28 ATOM 6616 N ASP 984 -10.106 11.5825 20.266 1.00 11.28 ATOM 6617 CA ASP 984 -10.106 11.5825 20.266 1.00 11.00 ATOM 6618 CB ASP 984 -10.106 11.5825 20.266 1.00 11.00 ATOM 6619 CC BEU 985 -10.537 -9.055 20.265 1.00 10.15 ATOM 6620 CD1 LEU 985 -10.537 -9.055 20.266 1.00 12.17 ATOM 6621 CD ALA 983 -7.460 11.304 11.595 1.00 11.64 ATOM 6622 CD ALA 983 -7.460 11.304 11.595 1.00 11.67 ATOM 6636 CC BEU 985 -10.537 -9.055 20.266 1.00 11.10 ATOM 6636 CC BEU 985 -10.537 -9.055 20.266 1.00 11.10 ATOM 6636 CC BEU 985 -10.537 -9.055 20.266 1.00 11.37 ATOM 6636 CC BEU 985 -10.537 -9.055 20.266 1.00 11.37 ATOM 6636 CC BEU 985 -10.537 -9.055 20.266 1.00 11.35 ATOM | | | | | | | | | |
| ATOM 6594 C LEU 980 -9.970 -19.627 8.604 1.00 11.62 ATOM 6595 N LEU 981 -9.187 -18.677 9.099 1.00 12.13 ATOM 6596 CA LEU 981 -9.187 -18.677 9.099 1.00 12.13 ATOM 6597 CB LEU 981 -7.132 -18.495 10.387 1.00 10.9 ATOM 6598 CC LEU 981 -7.132 -18.495 10.387 1.00 10.9 ATOM 6599 CD1 LEU 981 -4.741 -18.760 11.090 1.00 12.12 ATOM 6509 CD2 LEU 981 -4.741 -18.706 11.090 1.00 12.12 ATOM 6601 C LEU 981 -9.301 -17.827 11.448 1.00 10.37 ATOM 6601 C LEU 981 -9.301 -17.827 11.448 1.00 10.37 ATOM 6601 C LEU 981 -9.917 -16.604 11.321 1.00 15.27 ATOM 6602 O LEU 981 -9.994 -18.394 12.445 1.00 9.87 ATOM 6606 CG LEU 982 -10.604 -17.564 13.495 1.00 10.87 ATOM 6606 CG LEU 982 -19.984 -18.395 1.00 10.87 ATOM 6606 CG LEU 982 -19.488 13.095 1.00 13.85 ATOM 6607 CD1 LEU 982 -19.997 -18.480 13.095 1.00 13.85 ATOM 6608 CD2 LEU 982 -19.484 13.495 1.00 12.2 ATOM 6608 CD2 LEU 982 -19.997 -18.480 13.095 1.00 13.85 ATOM 6609 C LEU 982 -9.659 -17.532 14.675 1.00 12.49 ATOM 6610 C LEU 982 -9.659 -17.532 14.675 1.00 12.49 ATOM 6610 C LEU 982 -9.659 -17.532 14.675 1.00 12.49 ATOM 6610 C LEU 982 -9.659 -17.532 14.675 1.00 12.49 ATOM 6610 C LEU 982 -9.659 -17.532 14.675 1.00 12.49 ATOM 6610 C LEU 982 -9.659 -17.532 14.675 1.00 12.49 ATOM 6610 C A ALA 983 -9.579 -16.400 15.364 1.00 11.23 ATOM 6611 C A ALA 983 -9.579 -16.401 17.557 1.00 11.23 ATOM 6612 CA ALA 983 -9.455 1.676 17.682 1.00 19.95 ATOM 6613 CB ALA 983 -9.455 1.676 17.682 1.00 19.95 ATOM 6614 C ALA 983 -9.455 1.676 17.682 1.00 19.95 ATOM 6616 N ASP 984 -10.108 -16.871 11.498 1.00 12.30 ATOM 6617 CA ALA 983 -9.455 1.676 17.682 1.00 19.15 ATOM 6620 CD DL ASP 984 -10.108 -16.871 11.198 1.00 12.69 ATOM 6631 CB ALA 989 -9.455 1.676 17.682 1.00 19.01 ATOM 6630 CD DL SSP 984 -10.108 -16.871 11.198 1.00 12.60 ATOM 6631 CB ALA 989 -1.00 10.60 11.50 | | | | | | | | | |
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| ATOM 6596 CA LEU 981 -8.647 -18.760 10.447 1.00 9.55 ATOM 6597 CB LEU 981 -7.132 -18.495 10.387 1.00 10.94 ATOM 6598 CG LEU 981 -6.4741 -18.706 11.090 1.00 12.12 ATOM 6600 CD2 LEU 981 -6.472 -17.977 12.747 1.00 15.207 ATOM 6601 C LEU 981 -9.301 -17.827 11.448 1.00 10.37 ATOM 6602 C LEU 981 -9.301 -17.827 11.448 1.00 10.37 ATOM 6603 N LEU 982 -9.984 -18.394 12.445 1.00 10.37 ATOM 6606 CB LEU 982 -10.604 -17.564 13.485 1.00 10.37 ATOM 6606 CB LEU 982 -10.604 -17.564 13.485 1.00 10.37 ATOM 6606 CB LEU 982 -11.948 -18.140 13.951 1.00 12.12 ATOM 6606 CB LEU 982 -11.948 -18.140 13.951 1.00 12.12 ATOM 6607 CD1 LEU 982 -12.997 -18.480 11.715 1.00 13.63 ATOM 6608 CD2 LEU 982 -11.948 -18.140 13.951 1.00 13.63 ATOM 6609 C LEU 982 -12.997 -18.480 11.715 1.00 13.63 ATOM 6610 O LEU 982 -9.597 -18.480 11.715 1.00 13.63 ATOM 6610 C LEU 982 -9.597 -18.480 11.715 1.00 13.63 ATOM 6610 C LEU 982 -9.599 -17.531 14.675 1.00 12.23 ATOM 6611 N ALA 983 -9.579 -16.400 15.364 1.00 11.28 ATOM 6612 CA ALA 983 -9.579 -16.400 15.364 1.00 11.28 ATOM 6613 CB ALA 983 -9.579 -16.400 15.364 1.00 11.28 ATOM 6616 C A ALA 983 -9.579 -16.400 15.364 1.00 11.28 ATOM 6617 CA ASP 984 -10.108 -16.374 18.829 1.00 10.64 ATOM 6618 CB ASP 984 -10.108 -16.374 18.829 1.00 10.63 ATOM 6617 CA ASP 984 -10.108 -16.374 18.829 1.00 10.63 ATOM 6618 CB ASP 984 -10.108 -16.374 18.829 1.00 10.63 ATOM 6617 CA ASP 984 -10.108 -16.5825 20.026 1.00 1.00 ATOM 6618 CB ASP 984 -10.108 -16.5825 20.026 1.00 1.00 ATOM 6618 CB ASP 984 -10.108 -16.5825 20.026 1.00 1.00 ATOM 6620 CD ASP 984 -10.108 -16.5825 20.026 1.00 1.00 ATOM 6630 CC LEU 985 -10.051 -1.051 20.438 1.00 14.80 ATOM 6631 CD ASP 984 -10.108 -18.592 21.593 1.00 14.67 ATOM 6632 C A LEU 985 -10.051 -1.051 20.438 1.00 14.80 ATOM 6634 C PRO 986 -7.280 -12.891 23.695 1.00 10.62 ATOM 6636 C C LEU 985 -10.051 -1.051 20.439 1.00 10.62 ATOM 6636 C C LEU 985 -10.051 -1.051 20.439 1.00 10.52 ATOM 6636 C C LEU 985 -10.051 -1.051 20.439 1.00 10.52 ATOM 6636 C C LEU 985 -10.053 -1.051 20.595 1.00 10.62 ATOM 6636 C C PRO 986 -7.280 -1 | MOTA | 6594 | 0 | LEU | 980 | | | | |
| ATOM 6597 CB LEU 981 | MOTA | 6595 | N | LEU | 981 | -9.187 | -18.677 | 9.099 | 1.00 12.13 |
| ATOM 6598 CC LEU 981 -6.195 -18.853 11.539 1.00 12.12 ATOM 6500 CD2 LEU 981 -4.741 -18.706 11.090 1.00 12.07 ATOM 6601 C LEU 981 -6.472 -17.977 12.747 1.00 12.07 ATOM 6601 C LEU 981 -9.301 -17.827 11.448 1.00 10.37 ATOM 6602 C LEU 981 -9.301 -17.827 11.448 1.00 10.37 ATOM 6602 C LEU 981 -9.197 -16.604 11.321 1.00 11.18 ATOM 6603 N LEU 982 -19.984 -18.394 12.445 1.00 19.37 ATOM 6605 CB LEU 982 -10.604 -17.564 13.485 1.00 19.54 ATOM 6605 CB LEU 982 -11.948 18.140 13.951 1.00 12.12 ATOM 6606 CG LEU 982 -13.182 -17.868 13.095 1.00 13.63 ATOM 6606 CG LEU 982 -12.997 -18.480 11.715 1.00 12.12 ATOM 6608 CD2 LEU 982 -14.414 -18.442 13.792 1.00 14.38 ATOM 6609 C LEU 982 -9.659 -17.532 14.675 1.00 12.83 ATOM 6610 O LEU 982 -9.659 -17.532 14.675 1.00 12.83 ATOM 6610 O LEU 982 -9.659 -17.532 14.675 1.00 12.43 ATOM 6610 C LEU 982 -74.414 -18.424 13.792 1.00 14.38 ATOM 6611 N ALA 983 -9.579 -16.400 15.364 1.00 11.23 ATOM 6612 CA ALA 983 -9.579 -16.400 15.364 1.00 11.23 ATOM 6613 CB ALA 983 -7.440 -15.542 16.217 1.00 9.52 ATOM 6614 C ALA 983 -7.440 -15.542 16.217 1.00 9.55 ATOM 6616 N ASP 984 -9.455 -15.676 17.682 1.00 9.95 ATOM 6616 N ASP 984 -9.455 -15.676 17.682 1.00 10.15 ATOM 6617 CA ASP 984 -10.108 -16.871 21.148 1.00 11.03 ATOM 6619 CG ASP 984 -10.108 -16.871 21.148 1.00 14.80 ATOM 6619 CG ASP 984 -10.108 -16.871 21.148 1.00 14.80 ATOM 6620 ODI ASP 984 -10.108 -16.871 21.148 1.00 14.63 ATOM 6620 CDI ASP 984 -10.108 -16.871 21.148 1.00 14.08 ATOM 6620 CDI ASP 984 -10.108 -16.871 21.148 1.00 14.08 ATOM 6620 CDI ASP 984 -10.108 -16.871 21.148 1.00 14.08 ATOM 6630 C BEU 985 -10.537 -9.055 20.026 1.00 10.15 ATOM 6631 C BEU 985 -10.537 -9.055 20.026 1.00 10.15 ATOM 6630 C BEU 985 -10.537 -9.055 20.026 1.00 10.15 ATOM 6630 C BEU 985 -10.537 -9.055 20.056 1.00 10.15 ATOM 6630 C BEU 985 -10.537 -9.055 20.055 1.00 10.62 ATOM 6631 C BEU 985 -10.537 -9.055 20.055 1.00 10.10 10.70 ATOM 6631 C BEU 985 -10.537 -9.055 20.055 1.00 10.05 ATOM 6630 C BEU 985 -10.537 -9.055 20.055 1.00 10.52 ATOM 6630 C BEU 985 -10.537 -9.055 20.055 1.00 | MOTA | 6596 | CA | LEU | 981 | -8.647 | -18.760 | 10.447 | 1.00 9.55 |
| ATOM 6598 CG LEU 981 | MOTA | 6597 | CB | LEU | 981 | -7.132 | -18.495 | 10.387 | 1.00 10.99 |
| ATOM 6699 CD1 LEU 981 | | | | | | | -18.853 | | 1.00 12.12 |
| ATOM 6601 CD LEU 981 | | | | | | | | | |
| ATOM 6601 C LEU 981 -9.301 -17.827 11.448 1.00 10.37 ATOM 6602 C LEU 981 -9.197 -16.604 11.321 1.00 11.18 ATOM 6603 N LEU 982 -9.984 -18.394 12.445 1.00 9.54 ATOM 6605 CB LEU 982 -10.604 -17.564 13.485 1.00 10.87 ATOM 6605 CB LEU 982 -11.948 -18.104 13.951 1.00 12.12 ATOM 6605 CB LEU 982 -11.948 -18.104 13.951 1.00 12.12 ATOM 6606 CCD LEU 982 -11.948 -18.104 13.951 1.00 13.63 ATOM 6607 CD1 LEU 982 -12.997 -18.480 11.715 1.00 13.85 ATOM 6608 CD2 LEU 982 -12.997 -18.480 11.715 1.00 13.85 ATOM 6608 CD2 LEU 982 -14.414 -18.442 13.792 1.00 12.42 ATOM 6610 C LEU 982 -9.659 -17.532 14.675 1.00 12.49 ATOM 6610 C LEU 982 -8.891 -18.521 14.951 1.00 12.49 ATOM 6610 C LEU 982 -9.659 -17.532 14.675 1.00 12.63 ATOM 6611 N ALA 983 -9.579 -16.400 15.364 1.00 11.23 ATOM 6612 CA ALA 983 -9.579 -16.400 15.364 1.00 11.23 ATOM 6613 CB ALA 983 -9.579 -16.400 15.364 1.00 11.23 ATOM 6614 C ALA 983 -9.455 -15.676 17.682 1.00 9.52 ATOM 6615 O ALA 983 -9.455 -15.676 17.682 1.00 9.52 ATOM 6616 N ASP 984 -9.452 -16.347 18.829 1.00 10.15 ATOM 6617 CA ASP 984 -10.116 -15.825 20.026 1.00 11.05 ATOM 6618 CB ASP 984 -10.108 -16.871 21.148 1.00 14.08 ATOM 6619 CG ASP 984 -11.332 -17.763 21.159 1.00 16.37 ATOM 6620 CD ASP 984 -11.332 -17.763 21.159 1.00 16.37 ATOM 6621 ODZ ASP 984 -11.332 -17.763 21.159 1.00 16.37 ATOM 6620 CD ASP 984 -11.332 -17.763 21.159 1.00 16.37 ATOM 6620 CD ASP 984 -11.332 -17.763 21.159 1.00 10.62 ATOM 6620 CD ASP 984 -10.108 -16.871 21.148 1.00 14.08 ATOM 6620 CD ASP 984 -10.305 -17.478 20.438 1.00 14.08 ATOM 6620 CD ASP 984 -10.305 -17.478 20.438 1.00 14.08 ATOM 6620 CD ASP 984 -10.305 -17.478 20.438 1.00 14.08 ATOM 6620 CD ASP 984 -10.305 -17.478 20.438 1.00 14.08 ATOM 6620 CD ASP 984 -10.305 -17.478 20.438 1.00 14.08 ATOM 6620 CD ASP 984 -10.305 -17.478 20.438 1.00 14.09 ATOM 6620 CD ASP 985 -10.557 -9.055 20.695 1.00 10.12 ATOM 6630 CD ASP 986 -9.390 -14.627 20.595 1.00 10.62 ATOM 6630 CD ASP 986 -9.529 -12.587 21.864 1.00 10.32 ATOM 6631 CD EUU 985 -10.537 -9.055 20.695 1.00 10.12 ATOM 6630 CD ASP 986 -9.529 -12.587 | | | | | | | | | |
| ATOM 6602 O LEU 981 | | | | | | | | | |
| ATOM 6604 CA LEU 982 -9.984 -18.394 12.445 1.00 9.54 ATOM 6605 CB LEU 982 -10.604 -17.564 13.485 1.00 10.87 ATOM 6605 CB LEU 982 -11.948 -18.140 13.951 1.00 12.12 ATOM 6606 CG LEU 982 -13.182 -17.868 13.095 1.00 13.85 ATOM 6607 CD1 LEU 982 -12.997 -18.480 11.715 1.00 13.85 ATOM 6608 CD2 LEU 982 -12.997 -18.480 11.715 1.00 13.85 ATOM 6609 C LEU 982 -9.659 -17.532 14.675 1.00 12.63 ATOM 6610 D LEU 982 -9.659 -17.532 14.675 1.00 12.63 ATOM 6611 N ALA 983 -9.579 -16.400 15.364 1.00 11.23 ATOM 6612 CA ALA 983 -9.579 -16.400 15.364 1.00 12.63 ATOM 6613 CB ALA 983 -9.579 -16.400 15.364 1.00 12.63 ATOM 6614 C ALA 983 -9.455 -15.676 17.662 1.00 9.62 ATOM 6615 O ALA 983 -9.455 -15.676 17.662 1.00 9.62 ATOM 6616 N ASP 984 -10.108 -16.871 21.148 1.00 10.15 ATOM 6617 CA ASP 984 -10.108 -16.871 21.148 1.00 10.16 ATOM 6618 CB ASP 984 -10.108 -16.871 21.148 1.00 14.08 ATOM 6620 DD1 ASP 984 -11.332 -17.763 21.159 1.00 16.37 ATOM 6621 DD ASP 984 -11.332 -17.763 21.159 1.00 16.37 ATOM 6622 C ASP 984 -10.108 -16.871 21.148 1.00 14.08 ATOM 6623 N ASP 984 -10.304 -18.755 21.923 1.00 16.37 ATOM 6624 N LEU 985 -10.151 -13.688 21.137 1.00 16.37 ATOM 6625 CB LEU 985 -10.151 -13.688 21.137 1.00 16.37 ATOM 6626 CB LEU 985 -10.574 20.323 1.00 14.64 ATOM 6627 CG LEU 985 -10.537 -9.65 20.695 1.00 10.15 ATOM 6630 C LEU 985 -10.537 -9.65 20.695 1.00 10.17 ATOM 6628 CD1 LEU 985 -10.537 -9.65 20.695 1.00 10.18 ATOM 6630 C LEU 985 -10.537 -9.65 20.695 1.00 10.18 ATOM 6631 C DEU 985 -9.725 -13.204 23.247 1.00 10.73 ATOM 6632 C DPRO 986 -8.698 -13.302 25.015 1.00 10.52 ATOM 6634 C PRO 986 -9.309 -13.046 25.372 1.00 10.52 ATOM 6637 C PRO 986 -9.309 -13.046 25.372 1.00 10.53 ATOM 6636 CB PRO 986 -9.309 -13.046 25.372 1.00 10.53 ATOM 6637 C PRO 986 -9.309 -13.046 25.372 1.00 10.52 ATOM 6638 CD PRO 986 -9.309 -13.046 25.372 1.00 10.52 ATOM 6640 CD PRO 986 -9.309 -13.046 25.372 1.00 10.52 ATOM 6640 CD PRO 986 -9.309 -13.046 25.492 1.00 10.53 ATOM 6640 CD PRO 986 -9.309 -13.046 25.492 1.00 10.53 ATOM 6640 CD PRO 986 -9.309 -13.046 25.492 1.00 10.53 ATOM | | | | | | | | | |
| ATOM 6604 CA LEU 982 -10.604 -17.564 13.485 1.00 10.87 ATOM 6605 CB LEU 982 -13.182 -17.868 13.095 1.00 13.63 ATOM 6606 CG LEU 982 -12.997 -18.480 13.095 1.00 13.63 ATOM 6607 CD1 LEU 982 -12.997 -18.480 13.095 1.00 13.63 ATOM 6608 CD2 LEU 982 -12.997 -18.480 11.715 1.00 13.63 ATOM 6609 C LEU 982 -9.659 -17.532 14.675 1.00 12.49 ATOM 6610 O LEU 982 -8.991 -18.521 14.951 1.00 12.49 ATOM 6611 N ALA 983 -9.579 -16.400 15.364 1.00 11.23 ATOM 6612 CA ALA 983 -7.440 -15.542 16.217 1.00 9.62 ATOM 6613 CB ALA 983 -7.440 -15.542 16.217 1.00 9.62 ATOM 6616 N ASP 984 -9.455 -15.676 17.662 1.00 9.95 ATOM 6616 N ASP 984 -9.455 -15.676 17.662 1.00 10.15 ATOM 6617 CA ASP 984 -10.116 -15.825 20.026 1.00 11.00 ATOM 6618 CB ASP 984 -10.116 -15.825 20.026 1.00 16.37 ATOM 6620 OD1 ASP 984 -10.108 -16.871 21.148 1.00 14.80 ATOM 6621 OD2 ASP 984 -11.332 -17.763 21.159 1.00 16.37 ATOM 6622 C ASP 984 -11.304 -18.755 21.923 1.00 14.80 ATOM 6623 O ASP 984 -13.304 -18.755 21.923 1.00 16.37 ATOM 6624 N LEU 985 -9.9390 -14.627 20.592 1.00 10.15 ATOM 6625 CA LEU 985 -9.9390 -14.627 20.592 1.00 10.79 ATOM 6626 CB LEU 985 -10.513 -13.688 21.137 1.00 10.79 ATOM 6626 CB LEU 985 -10.513 -13.688 21.137 1.00 10.79 ATOM 6627 CB LEU 985 -10.529 -12.587 21.864 1.00 10.79 ATOM 6628 CD LEU 985 -10.513 -13.688 21.137 1.00 10.79 ATOM 6629 CD2 LEU 985 -10.537 -9.065 20.695 1.00 10.79 ATOM 6630 C LEU 985 -10.531 -10.542 20.024 1.00 10.79 ATOM 6631 C D PRO 986 -8.651 -13.315 24.034 1.00 10.79 ATOM 6632 C PRO 986 -8.698 -13.906 25.372 1.00 10.52 ATOM 6634 C PRO 986 -9.309 -11.298 23.695 1.00 10.53 ATOM 6637 C PRO 986 -9.725 -13.204 23.247 1.00 10.33 ATOM 6636 CG PRO 986 -9.309 -12.587 21.864 1.00 11.37 ATOM 6636 CG PRO 986 -9.309 -13.904 23.247 1.00 10.79 ATOM 6637 C PRO 986 -9.725 -13.204 23.247 1.00 10.79 ATOM 6638 C PRO 986 -9.725 -13.204 23.247 1.00 10.33 ATOM 6640 CB PRO 986 -9.309 -13.904 23.265 1.00 10.33 ATOM 6640 CB PRO 986 -9.309 -13.904 23.265 1.00 10.33 ATOM 6640 CB PRO 986 -9.309 -13.904 23.265 1.00 10.33 ATOM 6640 CB PRO 986 -9.309 -13.904 23.26 | | | | | | | | | |
| ATOM 6605 CB LEU 982 -11.948 -18.140 13.951 1.00 12.12 ATOM 6606 CG LEU 982 -12.997 -18.480 11.715 1.00 13.63 ATOM 6607 CD1 LEU 982 -12.997 -18.480 11.715 1.00 13.85 ATOM 6608 CD2 LEU 982 -14.414 -18.442 13.792 1.00 14.38 ATOM 6610 C LEU 982 -9.659 -17.532 14.951 1.00 12.49 ATOM 6611 N ALA 983 -9.579 -16.400 15.364 1.00 12.49 ATOM 6612 CA ALA 983 -9.579 -16.400 15.364 1.00 11.28 ATOM 6613 CB ALA 983 -9.455 -15.676 17.682 1.00 14.38 ATOM 6614 C ALA 983 -9.455 -15.676 17.682 1.00 9.95 ATOM 6615 O ALA 983 -9.455 -15.676 17.682 1.00 9.95 ATOM 6616 N ASP 984 -0.452 -16.347 18.829 1.00 10.15 ATOM 6617 CA ASP 984 -10.106 -15.825 20.026 1.00 11.00 ATOM 6618 CB ASP 984 -10.116 -15.825 20.026 1.00 11.00 ATOM 6619 CG ASP 984 -11.332 -17.763 21.148 1.00 14.80 ATOM 6620 DD1 ASP 984 -11.332 -17.763 21.148 1.00 14.80 ATOM 6621 CD2 ASP 984 -11.332 -17.763 20.252 1.00 16.62 ATOM 6622 C ASP 984 -11.304 -18.755 21.923 1.00 14.64 ATOM 6623 O ASP 984 -11.304 -18.755 21.923 1.00 14.64 ATOM 6624 N LEU 985 -10.151 -13.688 21.137 1.00 10.17 ATOM 6626 CB LEU 985 -10.537 -9.065 20.695 1.00 10.12 ATOM 6627 CG LEU 985 -10.537 -9.065 20.695 1.00 11.87 ATOM 6628 CD1 LEU 985 -10.537 -9.065 20.695 1.00 11.87 ATOM 6629 CD2 LEU 985 -10.537 -9.065 20.695 1.00 11.00 ATOM 6630 C LEU 985 -10.537 -9.065 20.695 1.00 16.64 ATOM 6630 C LEU 985 -10.537 -9.065 20.695 1.00 16.64 ATOM 6630 C LEU 985 -10.537 -9.065 20.695 1.00 16.64 ATOM 6630 C DEU 985 -10.537 -9.065 20.695 1.00 16.05 ATOM 6631 O LEU 985 -10.537 -9.065 20.695 1.00 16.00 12.35 ATOM 6632 C DPRO 986 -8.698 -13.906 25.372 1.00 16.33 ATOM 6634 C PRO 986 -9.309 -13.046 26.492 1.00 10.15 ATOM 6636 CB PRO 986 -9.309 -13.046 26.492 1.00 10.52 ATOM 6636 CB PRO 986 -9.309 -13.046 26.492 1.00 10.52 ATOM 6636 CB PRO 986 -9.309 -13.046 26.492 1.00 10.33 ATOM 6640 CB PRO 986 -9.309 -13.046 26.492 1.00 10.33 ATOM 6641 CB PRE 987 -9.725 -13.294 33.885 1.00 12.20 ATOM 6640 CB PRE 987 -9.726 -13.722 33.018 1.00 12.00 ATOM 6640 CB PRE 987 -9.726 -13.697 32.265 1.00 11.30 ATOM 6640 CB PRE 987 -9.726 -13.699 33.0 | MOTA | 6603 | N | LEU | | | | | |
| ATOM 6606 CG LEU 982 -13.182 -17.868 13.095 1.00 13.63 ATOM 6607 CD1 LEU 982 -12.997 -18.480 11.715 1.00 13.63 ATOM 6608 CD2 LEU 982 -14.414 -18.442 13.792 1.00 14.38 ATOM 6609 C LEU 982 -9.659 -17.532 14.675 1.00 12.49 ATOM 6610 O LEU 982 -8.991 -18.521 14.951 1.00 12.49 ATOM 6611 N ALA 983 -9.579 -16.400 15.364 1.00 11.23 ATOM 6612 CA ALA 983 -9.579 -16.400 15.364 1.00 11.23 ATOM 6613 CB ALA 983 -9.455 -16.324 16.533 1.00 11.28 ATOM 6616 CB ALA 983 -9.455 -15.676 17.682 1.00 9.95 ATOM 6617 CA ALA 983 -9.455 -15.676 17.682 1.00 9.95 ATOM 6616 N ASP 984 -9.452 -16.347 18.829 1.00 10.15 ATOM 6617 CA ASP 984 -10.116 -15.825 20.026 1.00 11.00 ATOM 6618 CB ASP 984 -10.116 -15.825 20.026 1.00 11.00 ATOM 6620 OD1 ASP 984 -11.332 -17.763 21.159 1.00 16.37 ATOM 6621 OD2 ASP 984 -11.332 -17.763 21.159 1.00 16.37 ATOM 6620 OD2 ASP 984 -11.332 -17.763 21.159 1.00 16.63 ATOM 6621 OD2 ASP 984 -11.304 -18.755 21.923 1.00 14.60 ATOM 6623 O ASP 984 -12.305 -17.478 20.438 1.00 14.80 ATOM 6624 N LEU 985 -9.529 -12.587 21.864 1.00 10.77 ATOM 6626 CB LEU 985 -9.529 -12.587 21.864 1.00 10.77 ATOM 6626 CB LEU 985 -9.529 -12.587 21.864 1.00 11.87 ATOM 6627 CG LEU 985 -10.051 -13.688 21.137 1.00 10.79 ATOM 6630 C LEU 985 -10.051 -13.688 21.137 1.00 10.79 ATOM 6631 O LEU 985 -10.537 -9.065 20.695 1.00 10.62 ATOM 6632 N PRO 986 -8.613 -10.542 20.102 1.00 17.01 ATOM 6633 C LEU 985 -10.537 -9.065 20.695 1.00 10.52 ATOM 6634 N PRO 986 -8.698 -13.906 25.372 1.00 10.52 ATOM 6635 CB PRO 986 -9.725 -13.204 23.247 1.00 10.75 ATOM 6636 CG PRO 986 -9.725 -13.204 23.247 1.00 10.75 ATOM 6637 C PRO 986 -9.725 -13.204 23.247 1.00 10.33 ATOM 6638 O PRO 986 -9.725 -13.204 23.247 1.00 10.33 ATOM 6640 CD PRE 987 -9.939 -12.891 23.695 1.00 10.33 ATOM 6641 CB PRE 987 -9.939 -12.984 31.418 1.00 10.30 ATOM 6642 CG PRE 987 -9.939 -12.984 31.418 1.00 10.30 ATOM 6645 CE PRE 987 -9.952 -12.993 31.421 25.633 1.00 12.21 ATOM 6646 CC PRE 987 -9.970 -12.984 31.418 1.00 10.30 ATOM 6646 CC PRE 987 -9.970 -12.984 31.418 1.00 10.30 ATOM 6646 CC PRE 987 -9.970 -12.984 31 | MOTA | 6604 | CA | LEU | 982 | -10.604 | -17.564 | 13.485 | 1.00 10.87 |
| ATOM 6608 CD2 LEU 982 -12.997 -18.480 11.715 1.00 13.85 ATOM 6608 CD2 LEU 982 -14.414 -18.442 13.792 1.00 14.38 ATOM 6609 C LEU 982 -9.659 -17.532 14.675 1.00 12.49 ATOM 6610 O LEU 982 -8.991 -18.521 14.675 1.00 12.49 ATOM 6611 N ALA 983 -9.579 -16.400 15.364 1.00 11.28 ATOM 6612 CA ALA 983 -8.715 -16.324 16.533 1.00 11.28 ATOM 6613 CB ALA 983 -9.579 -16.400 15.542 16.217 1.00 9.62 ATOM 6614 C ALA 983 -9.455 -15.676 17.682 1.00 9.62 ATOM 6615 O ALA 983 -9.455 -15.676 17.682 1.00 9.5 ATOM 6616 N ASP 984 -9.452 -16.347 18.829 1.00 11.28 ATOM 6616 N ASP 984 -9.452 -16.347 18.829 1.00 11.05 ATOM 6617 CA ASP 984 -10.116 -15.825 20.026 1.00 11.05 ATOM 6619 CG ASP 984 -10.108 -16.871 21.148 1.00 14.08 ATOM 6619 CG ASP 984 -11.332 -17.763 21.159 1.00 14.08 ATOM 6620 ODJ ASP 984 -11.332 -17.763 21.159 1.00 14.08 ATOM 6620 ODJ ASP 984 -11.332 -17.478 20.438 1.00 14.64 ATOM 6622 C ASP 984 -11.304 -18.755 21.923 1.00 14.64 ATOM 6623 O ASP 984 -11.304 -18.755 21.923 1.00 14.64 ATOM 6623 O ASP 984 -11.304 -18.755 21.923 1.00 14.64 ATOM 6625 CA LEU 985 -9.529 -12.587 21.864 1.00 10.79 ATOM 6626 CD LEU 985 -10.151 -13.688 21.137 1.00 10.79 ATOM 6626 CD LEU 985 -9.529 -12.587 21.864 1.00 11.87 ATOM 6626 CD LEU 985 -10.537 -9.065 20.695 1.00 10.79 ATOM 6630 C LEU 985 -9.529 -12.587 21.864 1.00 11.87 ATOM 6620 CD LEU 985 -9.725 -13.204 23.247 1.00 11.87 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.79 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.79 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.75 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.75 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.37 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.35 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.55 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.35 ATOM 6630 C PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6637 C PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6634 C PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6634 C PRO 986 -9.721 -11.994 26.255 1.00 10.33 ATOM 6640 C PRE 987 -9.736 -13.204 23.265 1.00 10.30 | MOTA | 6605 | CB | LEU | 982 | -11.948 | -18.140 | 13.951 | 1.00 12.12 |
| ATOM 6608 CD2 LEU 982 -12.997 -18.480 11.715 1.00 13.85 ATOM 6608 CD2 LEU 982 -14.414 -18.442 13.792 1.00 14.38 ATOM 6609 C LEU 982 -9.659 -17.532 14.675 1.00 12.49 ATOM 6610 O LEU 982 -8.991 -18.521 14.951 1.00 12.63 ATOM 6611 N ALA 983 -9.579 -16.400 15.364 1.00 11.28 ATOM 6612 CA ALA 983 -8.715 -16.324 16.533 1.00 11.28 ATOM 6613 CB ALA 983 -8.715 -16.324 16.533 1.00 11.28 ATOM 6614 C ALA 983 -9.455 -15.676 17.682 1.00 9.62 ATOM 6615 O ALA 983 -9.455 -15.676 17.682 1.00 9.56 ATOM 6616 N ASP 984 -9.452 -16.347 18.829 1.00 11.04 ATOM 6616 N ASP 984 -10.106 -15.825 20.026 1.00 11.05 ATOM 6617 CA ASP 984 -10.108 -16.871 21.148 1.00 14.08 ATOM 6619 CG ASP 984 -11.332 -17.763 21.159 1.00 14.08 ATOM 6620 ODJ ASP 984 -11.332 -17.763 21.159 1.00 14.08 ATOM 6621 ODZ ASP 984 -11.332 -17.763 21.159 1.00 14.64 ATOM 6622 C ASP 984 -11.304 -18.755 21.923 1.00 14.64 ATOM 6623 O ASP 984 -11.304 -18.755 21.923 1.00 14.64 ATOM 6623 O ASP 984 -11.304 -18.755 21.923 1.00 14.64 ATOM 6623 O ASP 984 -11.304 -18.755 21.923 1.00 10.79 ATOM 6626 CB LEU 985 -9.529 -12.587 21.864 1.00 10.79 ATOM 6626 CB LEU 985 -9.529 -12.587 21.864 1.00 10.79 ATOM 6626 CB LEU 985 -9.529 -12.587 21.864 1.00 10.79 ATOM 6626 CB LEU 985 -9.529 -12.587 21.864 1.00 12.83 ATOM 6626 CB LEU 985 -9.529 -12.587 21.664 1.00 12.83 ATOM 6630 C LEU 985 -9.529 -10.510 20.479 1.00 14.09 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.05 1.34 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.05 1.34 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.05 1.34 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.05 1.34 ATOM 6630 C PRO 986 -7.280 -12.891 23.695 1.00 10.52 ATOM 6630 C PRO 986 -9.721 -11.914 26.255 1.00 10.53 ATOM 6630 C PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6630 C PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6634 C PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6640 C PRE 987 -9.736 -13.042 23.485 1.00 12.25 ATOM 6645 C PRE 987 -9.736 -13.204 23.8 | ATOM | 6606 | CG | LEU | 982 | -13.182 | -17.868 | 13.095 | 1.00 13.63 |
| ATOM 6609 C LEU 982 -14.414 -18.442 13.792 1.00 14.38 ATOM 6609 C LEU 982 -9.659 -17.532 14.675 1.00 12.49 ATOM 6610 O LEU 982 -8.991 -18.521 14.951 1.00 12.63 ATOM 6611 N ALA 983 -9.579 -16.400 15.364 1.00 11.23 ATOM 6612 CA ALA 983 -8.715 -16.324 16.533 1.00 11.28 ATOM 6613 CB ALA 983 -7.440 -15.542 16.217 1.00 9.62 ATOM 6614 C ALA 983 -9.455 -15.676 17.682 1.00 9.55 ATOM 6615 O ALA 983 -9.455 -15.676 17.682 1.00 9.95 ATOM 6616 N ASP 984 -9.452 -16.347 18.829 1.00 10.15 ATOM 6616 N ASP 984 -10.116 -15.825 20.026 1.00 11.00 ATOM 6618 CB ASP 984 -10.116 -15.825 20.026 1.00 11.00 ATOM 6619 CG ASP 984 -11.332 -17.763 21.159 1.00 16.37 ATOM 6620 OD1 ASP 984 -12.305 -17.478 20.438 1.00 14.80 ATOM 6621 OD2 ASP 984 -11.304 -18.755 21.923 1.00 14.80 ATOM 6622 C ASP 984 -11.304 -18.755 21.923 1.00 10.15 ATOM 6624 N LEU 985 -10.151 -13.688 21.137 1.00 10.79 ATOM 6626 CB LEU 985 -9.529 -12.587 21.864 1.00 10.77 ATOM 6626 CB LEU 985 -9.529 -12.587 21.864 1.00 11.87 ATOM 6627 CG LEU 985 -9.529 -12.587 21.864 1.00 12.83 ATOM 6628 CD1 LEU 985 -10.323 -11.259 21.763 1.00 12.83 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 10.52 ATOM 6631 O LEU 985 -10.337 -9.065 20.695 1.00 16.57 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 12.83 ATOM 6633 CD PRO 986 -7.280 -13.291 25.015 1.00 12.75 ATOM 6634 CA PRO 986 -8.698 -13.292 25.055 1.00 10.52 ATOM 6635 CB PRO 986 -9.725 -13.204 23.247 1.00 10.52 ATOM 6636 CG PRO 986 -9.725 -13.204 23.247 1.00 10.52 ATOM 6637 C PRO 986 -9.725 -13.204 23.247 1.00 10.52 ATOM 6638 CD PRO 986 -9.725 -13.204 23.247 1.00 10.52 ATOM 6639 N PHE 987 -9.939 -13.046 26.482 1.00 10.33 ATOM 6636 CG PRO 986 -9.729 -12.587 21.864 1.00 12.25 ATOM 6641 CB PHE 987 -9.939 -13.046 26.482 1.00 10.33 ATOM 6642 CD PRO 986 -9.309 -13.046 26.482 1.00 10.33 ATOM 6646 CC PRO 986 -9.909 -13.046 26.482 1.00 10.33 ATOM 6646 CC PRO 986 -9.309 -13.046 26.482 1.00 10.33 ATOM 6646 CD PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6646 CD PRE 987 -9.913 -12.938 28.856 1.00 11.35 ATOM 6646 CD PRE 987 -9.913 -12.697 33.265 1.00 11.35 | | 6607 | | | 982 | | | | 1.00 13.85 |
| ATOM 6609 C LEU 982 | | | | | | | | | |
| ATOM 6610 O LEU 982 | | | | | | | | | |
| ATOM 6611 N ALA 983 -9.579 -16.400 15.364 1.00 11.23 ATOM 6612 CA ALA 983 -8.715 -16.324 16.217 1.00 9.95 ATOM 6613 CB ALA 983 -7.440 -15.542 16.217 1.00 9.95 ATOM 6614 C ALA 983 -7.440 -15.542 16.217 1.00 9.95 ATOM 6615 O ALA 983 -9.455 -15.676 17.682 1.00 11.64 ATOM 6616 N ASP 984 -9.452 -16.347 18.829 1.00 11.64 ATOM 6617 CA ASP 984 -10.116 -15.825 20.026 1.00 11.00 ATOM 6618 CB ASP 984 -10.116 -15.825 20.026 1.00 11.00 ATOM 6619 CG ASP 984 -11.332 -17.763 21.148 1.00 14.08 ATOM 6620 OD1 ASP 984 -11.332 -17.763 21.159 1.00 16.37 ATOM 6621 OD2 ASP 984 -11.304 -18.755 21.923 1.00 14.80 ATOM 6622 C ASP 984 -11.304 -18.755 21.923 1.00 14.64 ATOM 6623 O ASP 984 -9.390 -14.627 20.592 1.00 10.62 ATOM 6625 CA LEU 985 -9.529 -12.587 21.864 1.00 10.17 ATOM 6626 CB LEU 985 -10.323 -11.295 21.763 1.00 12.83 ATOM 6627 CG LEU 985 -10.537 -9.055 20.695 1.00 11.80 ATOM 6630 C LEU 985 -10.537 -9.055 20.695 1.00 11.00 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.70 ATOM 6630 C LEU 985 -10.537 -9.055 20.695 1.00 16.64 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.91 ATOM 6631 O LEU 985 -10.837 -9.055 20.695 1.00 11.91 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 12.53 ATOM 6633 CD PRO 986 -7.280 -12.891 23.695 1.00 12.53 ATOM 6634 CA PRO 986 -8.658 -13.300 25.075 1.00 12.53 ATOM 6635 CB PRO 986 -9.725 -13.204 23.247 1.00 11.35 ATOM 6636 CB PRO 986 -9.728 -14.212 25.633 1.00 12.27 ATOM 6637 C PRO 986 -9.728 -14.221 25.633 1.00 12.27 ATOM 6638 O PRO 986 -9.728 -14.221 25.633 1.00 12.27 ATOM 6637 C PRO 986 -9.728 -14.221 25.633 1.00 12.27 ATOM 6638 O PRO 986 -9.721 -11.914 26.255 1.00 10.31 ATOM 6641 CB PHE 987 -9.941 -12.938 28.856 1.00 10.31 ATOM 6641 CB PHE 987 -9.954 -13.3046 26.482 1.00 10.32 ATOM 6640 CA PHE 987 -9.954 -13.3046 26.482 1.00 10.31 ATOM 6641 CB PHE 987 -9.954 -13.3046 26.482 1.00 10.31 ATOM 6640 CB PHE 987 -9.954 -13.3046 26.482 1.00 10.31 ATOM 6641 CB PHE 987 -9.954 -13.3046 26.482 1.00 10.31 ATOM 6646 CE2 PHE 987 -9.956 -12.2984 31.418 1.00 11.30 | | | | | | | | | |
| ATOM 6612 CA ALA 983 | | | | | | | | | |
| ATOM 6613 CB ALA 983 | | | | | | | | | |
| ATOM 6614 C ALA 983 | ATOM | | | | | | | | |
| ATOM 6615 O ALA 983 | MOTA | 6613 | CB | ALA | 983 | | | | |
| ATOM 6616 N ASP 984 -9.452 -16.347 18.829 1.00 10.15 ATOM 6617 CA ASP 984 -10.116 -15.825 20.026 1.00 11.00 ATOM 6618 CB ASP 984 -10.108 -16.871 21.148 1.00 14.08 ATOM 6619 CG ASP 984 -11.332 -17.763 21.159 1.00 16.37 ATOM 6620 OD1 ASP 984 -11.332 -17.763 21.159 1.00 14.80 ATOM 6621 OD2 ASP 984 -11.304 -18.755 21.923 1.00 14.64 ATOM 6622 C ASP 984 -9.390 -14.627 20.592 1.00 10.62 ATOM 6623 O ASP 984 -9.390 -14.627 20.592 1.00 10.62 ATOM 6624 N LEU 985 -10.151 -13.688 21.137 1.00 10.77 ATOM 6625 CA LEU 985 -9.529 -12.587 21.864 1.00 11.87 ATOM 6626 CB LEU 985 -10.323 -11.295 21.763 1.00 12.83 ATOM 6627 CG LEU 985 -10.537 -9.065 20.695 1.00 14.09 ATOM 6628 CD1 LEU 985 -10.537 -9.065 20.695 1.00 16.64 ATOM 6629 CD2 LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6631 O LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 12.35 ATOM 6633 CD PRO 986 -7.228 -14.291 25.633 1.00 12.55 ATOM 6634 CA PRO 986 -7.228 -14.291 25.633 1.00 12.55 ATOM 6635 CB PRO 986 -7.238 -14.221 25.633 1.00 12.21 ATOM 6636 CG PRO 986 -9.721 -11.914 26.255 1.00 10.32 ATOM 6637 C PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6638 O PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6639 N PHE 987 -9.524 -13.722 30.118 1.00 10.33 ATOM 6640 CA PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6642 CG PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6643 CD1 PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6644 CD2 PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6645 CE1 PHE 987 -9.524 -13.699 33.054 1.00 13.41 ATOM 6646 CE2 PHE 987 -9.570 -12.984 31.418 1.00 13.34 ATOM 6647 CZ PHE 987 -9.524 -13.724 33.885 1.00 13.88 ATOM 6649 O PHE 987 -11.272 -11.999 33.054 1.00 13.81 ATOM 6649 CP PHE 987 -10.196 -11.724 33.885 1.00 13.88 | MOTA | 6614 | C | ALA | 983 | -9.455 | -15.676 | 17.682 | 1.00 9.95 |
| ATOM 6617 CA ASP 984 -10.116 -15.825 20.026 1.00 11.00 ATOM 6618 CB ASP 984 -10.108 -16.871 21.148 1.00 14.08 ATOM 6619 CG ASP 984 -11.332 -17.763 21.159 1.00 16.37 ATOM 6620 OD1 ASP 984 -12.305 -17.478 20.438 1.00 14.80 ATOM 6621 OD2 ASP 984 -12.305 -17.478 20.438 1.00 14.80 ATOM 6622 C ASP 984 -9.390 -14.627 20.592 1.00 10.62 ATOM 6623 O ASP 984 -8.161 -14.538 20.524 1.00 10.17 ATOM 6624 N LEU 985 -10.151 -13.688 21.137 1.00 10.79 ATOM 6625 CA LEU 985 -9.529 -12.587 21.864 1.00 11.87 ATOM 6626 CB LEU 985 -10.323 -11.295 21.763 1.00 12.83 ATOM 6627 CG LEU 985 -10.537 -9.065 20.695 1.00 14.64 ATOM 6628 CD1 LEU 985 -10.537 -9.065 20.695 1.00 14.64 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6631 O LEU 985 -10.840 -13.590 23.606 1.00 12.15 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 12.35 ATOM 6633 CD PRO 986 -8.651 -13.315 24.034 1.00 12.35 ATOM 6634 CA PRO 986 -8.651 -13.315 24.034 1.00 12.35 ATOM 6635 CB PRO 986 -7.238 -14.221 25.633 1.00 12.21 ATOM 6636 CG PRO 986 -9.309 -13.046 26.482 1.00 10.52 ATOM 6637 C PRO 986 -9.309 -13.046 26.482 1.00 10.52 ATOM 6638 O PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6639 N PHE 987 -9.936 -13.614 27.684 1.00 10.33 ATOM 6640 CA PHE 987 -9.952 -12.984 31.418 1.00 10.31 ATOM 6641 CB PHE 987 -9.524 -13.722 33.695 1.00 10.33 ATOM 6642 CG PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6645 CEI PHE 987 -9.524 -13.722 33.695 1.00 10.31 ATOM 6646 CE2 PHE 987 -9.524 -13.722 33.695 1.00 10.31 ATOM 6647 CZ PHE 987 -9.524 -13.722 33.695 1.00 10.31 ATOM 6648 CDI PHE 987 -9.524 -13.722 33.695 1.00 10.31 ATOM 6646 CE2 PHE 987 -9.524 -13.722 33.695 1.00 13.41 ATOM 6646 CE2 PHE 987 -9.524 -13.724 33.895 1.00 13.84 ATOM 6646 CE2 PHE 987 -9.524 -13.724 33.895 1.00 13.88 ATOM 6647 CZ PHE 987 -11.272 -11.999 33.054 1.00 13.88 ATOM 6648 C PHE 987 -9.912 -11.294 23.8955 1.00 13.88 ATOM 6649 O PHE 987 -10.916 -11.724 33.895 1.00 13.88 ATOM 6649 O PHE 987 -10.916 -11.724 33.895 1.00 13.88 | MOTA | 6615 | 0 | ALA | 983 | -10.043 | -14.601 | 17.537 | 1.00 11.64 |
| ATOM 6617 CA ASP 984 -10.116 -15.825 20.026 1.00 11.00 ATOM 6618 CB ASP 984 -10.108 -16.871 21.148 1.00 14.08 ATOM 6620 OD1 ASP 984 -11.332 -17.763 21.159 1.00 16.37 ATOM 6621 OD2 ASP 984 -12.305 -17.478 20.438 1.00 14.80 ATOM 6621 OD2 ASP 984 -12.305 -17.478 20.438 1.00 14.80 ATOM 6622 C ASP 984 -11.304 -18.755 21.923 1.00 14.64 ATOM 6623 O ASP 984 -8.161 -14.538 20.524 1.00 10.17 ATOM 6624 N LEU 985 -10.151 -13.688 21.137 1.00 10.79 ATOM 6625 CA LEU 985 -9.529 -12.587 21.864 1.00 11.87 ATOM 6626 CB LEU 985 -10.323 -11.295 21.763 1.00 12.83 ATOM 6627 CG LEU 985 -10.537 -9.065 20.695 1.00 16.64 ATOM 6628 CD1 LEU 985 -10.537 -9.065 20.695 1.00 16.64 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6631 O LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 12.15 ATOM 6633 CD PRO 986 -8.651 -13.315 24.034 1.00 12.31 ATOM 6634 CA PRO 986 -8.651 -13.315 24.034 1.00 12.32 ATOM 6635 CB PRO 986 -7.238 -14.221 25.633 1.00 12.21 ATOM 6636 CG PRO 986 -9.721 -11.914 26.255 1.00 10.52 ATOM 6637 C PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6638 O PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6639 N PHE 987 -9.936 -13.614 27.684 1.00 10.33 ATOM 6640 CA PHE 987 -9.952 -12.984 31.418 1.00 10.31 ATOM 6641 CB PHE 987 -9.952 -12.999 33.054 1.00 11.95 ATOM 6647 CE PHE 987 -9.524 -13.722 33.493 1.00 12.08 ATOM 6647 CE PHE 987 -9.952 -12.999 33.054 1.00 10.31 ATOM 6647 CE PHE 987 -9.970 -12.984 31.418 1.00 10.30 ATOM 6647 CE PHE 987 -9.952 -12.697 32.265 1.00 10.31 ATOM 6647 CE PHE 987 -9.970 -12.984 31.418 1.00 10.30 ATOM 6647 CE PHE 987 -9.970 -12.984 31.418 1.00 10.30 ATOM 6647 CE PHE 987 -9.970 -12.984 31.418 1.00 10.30 ATOM 6648 CP PHE 987 -9.970 -12.994 31.418 1.00 12.08 ATOM 6647 CE PHE 987 -9.970 -12.994 31.418 1.00 13.84 ATOM 6648 CP PHE 987 -9.970 -12.994 31.418 1.00 13.88 ATOM 6649 O PHE 987 -10.196 -11.724 33.885 1.00 13.88 | ATOM | 6616 | N | ASP | 984 | -9.452 | -16.347 | 18.829 | 1.00 10.15 |
| ATOM 6618 CB ASP 984 -10.108 -16.871 21.148 1.00 14.08 ATOM 6619 CG ASP 984 -11.332 -17.763 21.159 1.00 16.37 ATOM 6620 OD1 ASP 984 -12.305 -17.478 20.438 1.00 14.80 ATOM 6621 OD2 ASP 984 -11.304 -18.755 21.923 1.00 14.64 ATOM 6622 C ASP 984 -9.390 -14.627 20.592 1.00 10.62 ATOM 6623 O ASP 984 -8.161 -14.538 20.524 1.00 10.17 ATOM 6624 N LEU 985 -10.151 -13.688 21.137 1.00 10.79 ATOM 6625 CA LEU 985 -9.529 -12.587 21.864 1.00 11.87 ATOM 6626 CB LEU 985 -9.529 -12.587 21.864 1.00 11.87 ATOM 6627 CG LEU 985 -10.323 -11.295 21.763 1.00 12.83 ATOM 6628 CD1 LEU 985 -10.537 -9.065 20.695 1.00 14.69 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 17.01 ATOM 6631 O LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 12.15 ATOM 6633 CD PRO 986 -8.651 -13.315 24.034 1.00 10.32 ATOM 6634 CA PRO 986 -8.651 -13.315 24.034 1.00 10.52 ATOM 6635 CB PRO 986 -7.280 -12.891 23.695 1.00 10.52 ATOM 6636 CG PRO 986 -7.280 -12.891 23.695 1.00 10.52 ATOM 6637 C PRO 986 -9.309 -13.046 25.372 1.00 12.27 ATOM 6638 O PRO 986 -9.309 -13.046 26.482 1.00 12.27 ATOM 6639 N PHE 987 -9.913 -12.938 28.856 1.00 10.33 ATOM 6630 C PRO 986 -9.309 -13.046 26.482 1.00 10.33 ATOM 6640 CA PHE 987 -9.954 -13.722 30.118 1.00 10.30 ATOM 6640 CB PHE 987 -9.524 -13.722 30.118 1.00 10.31 ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 10.31 ATOM 6645 CEI PHE 987 -9.524 -13.722 30.118 1.00 10.31 ATOM 6646 CE2 PHE 987 -9.770 -12.984 31.418 1.00 10.30 ATOM 6647 CZ PHE 987 -9.524 -13.722 33.493 1.00 12.20 ATOM 6648 CD PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6646 CE2 PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6647 CZ PHE 987 -9.770 -12.984 31.418 1.00 11.02 ATOM 6648 CD PHE 987 -9.770 -12.984 31.418 1.00 11.02 ATOM 6647 CZ PHE 987 -9.770 -12.984 31.418 1.00 11.02 ATOM 6648 CD PHE 987 -9.770 -12.984 31.418 1.00 11.02 ATOM 6649 CD PHE 987 -9.705 -12.697 33.493 1.00 12.09 ATOM 6649 CD PHE 987 -9.706 -11.724 33.885 1.00 13.88 | | | | | | -10.116 | -15.825 | 20.026 | 1.00 11.00 |
| ATOM 6619 CG ASP 984 -11.332 -17.763 21.159 1.00 16.37 ATOM 6620 OD1 ASP 984 -12.305 -17.478 20.438 1.00 14.80 ATOM 6621 OD2 ASP 984 -11.304 -18.755 21.923 1.00 14.64 ATOM 6622 C ASP 984 -9.390 -14.627 20.592 1.00 10.62 ATOM 6623 O ASP 984 -8.161 -14.538 20.524 1.00 10.17 ATOM 6624 N LEU 985 -10.151 -13.688 21.137 1.00 10.79 ATOM 6625 CA LEU 985 -9.529 -12.587 21.864 1.00 11.87 ATOM 6626 CB LEU 985 -9.529 -12.587 21.864 1.00 11.87 ATOM 6627 CG LEU 985 -10.091 -10.510 20.479 1.00 14.09 ATOM 6628 CD1 LEU 985 -10.537 -9.065 20.695 1.00 16.64 ATOM 6629 CD2 LEU 985 -8.613 -10.542 20.102 1.00 17.01 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6631 O LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 10.32 ATOM 6633 CD PRO 986 -8.651 -13.315 24.034 1.00 10.52 ATOM 6634 CA PRO 986 -8.698 -13.906 25.372 1.00 11.35 ATOM 6635 CB PRO 986 -6.563 -13.023 25.015 1.00 10.52 ATOM 6636 CG PRO 986 -6.563 -13.023 25.015 1.00 12.21 ATOM 6637 C PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6638 O PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6639 N PHE 987 -9.913 -12.938 28.856 1.00 10.31 ATOM 6640 CA PHE 987 -9.9524 -13.722 30.118 1.00 10.30 ATOM 6641 CB PHE 987 -9.9524 -13.722 30.118 1.00 12.08 ATOM 6647 CZ PHE 987 -9.770 -12.984 31.418 1.00 10.30 ATOM 6646 CE2 PHE 987 -9.770 -12.994 33.054 1.00 11.95 ATOM 6647 CZ PHE 987 -9.770 -12.999 33.054 1.00 12.08 ATOM 6648 C PHE 987 -9.770 -12.999 33.054 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.910 -12.070 33.493 1.00 12.08 ATOM 6647 CZ PHE 987 -9.9421 -11.491 28.955 1.00 11.02 ATOM 6648 C PHE 987 -9.9421 -11.491 28.955 1.00 13.88 ATOM 6648 C PHE 987 -9.9421 -11.491 28.955 1.00 13.88 | | | | | | | | | 1.00 14.08 |
| ATOM 6620 OD1 ASP 984 -12.305 -17.478 20.438 1.00 14.80 ATOM 6621 OD2 ASP 984 -11.304 -18.755 21.923 1.00 14.64 ATOM 6622 C ASP 984 -9.390 -14.627 20.592 1.00 10.62 ATOM 6623 O ASP 984 -8.161 -14.538 20.524 1.00 10.17 ATOM 6624 N LEU 985 -10.151 -13.688 21.137 1.00 10.79 ATOM 6625 CA LEU 985 -9.529 -12.587 21.864 1.00 11.87 ATOM 6626 CB LEU 985 -10.323 -11.295 21.763 1.00 12.83 ATOM 6627 CG LEU 985 -10.091 -10.510 20.479 1.00 14.09 ATOM 6628 CD1 LEU 985 -10.537 -9.065 20.695 1.00 14.64 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 17.01 ATOM 6631 O LEU 985 -9.725 -13.204 23.247 1.00 11.91 ATOM 6631 O LEU 985 -10.840 -13.590 23.606 1.00 12.15 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 12.15 ATOM 6633 CD PRO 986 -8.651 -13.315 24.034 1.00 10.32 ATOM 6635 CB PRO 986 -7.280 -12.891 23.695 1.00 10.52 ATOM 6636 CG PRO 986 -7.280 -12.891 23.695 1.00 10.52 ATOM 6636 CG PRO 986 -6.563 -13.023 25.015 1.00 12.75 ATOM 6637 C PRO 986 -6.563 -13.023 25.015 1.00 12.75 ATOM 6638 O PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6639 N PHE 987 -9.364 -13.512 24.324 1.00 10.33 ATOM 6634 CB PRO 986 -9.309 -13.046 26.482 1.00 10.33 ATOM 6634 CB PRO 986 -9.309 -13.046 26.482 1.00 10.33 ATOM 6640 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6640 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6640 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6640 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6645 CE2 PHE 987 -9.700 -12.984 31.418 1.00 10.30 ATOM 6646 CE2 PHE 987 -9.700 -12.984 31.418 1.00 10.30 ATOM 6646 CE2 PHE 987 -9.700 -12.984 31.418 1.00 10.30 ATOM 6646 CE2 PHE 987 -9.700 -12.994 33.054 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6648 C PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6648 C PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6648 C PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6649 O PHE 987 -8.910 -12.070 33.493 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 13.88 ATOM 6649 O PHE 987 -9.6421 -11.491 28.955 1.00 13.88 | | | | | | | | | |
| ATOM 6621 OD2 ASP 984 -11.304 -18.755 21.923 1.00 14.64 ATOM 6622 C ASP 984 -9.390 -14.627 20.592 1.00 10.62 ATOM 6623 O ASP 984 -8.161 -14.538 20.524 1.00 10.17 ATOM 6624 N LEU 985 -10.151 -13.688 21.137 1.00 10.79 ATOM 6625 CA LEU 985 -9.529 -12.587 21.864 1.00 11.87 ATOM 6626 CB LEU 985 -10.323 -11.295 21.763 1.00 12.83 ATOM 6627 CG LEU 985 -10.091 -10.510 20.479 1.00 14.09 ATOM 6628 CD1 LEU 985 -10.537 -9.065 20.695 1.00 16.64 ATOM 6630 C LEU 985 -8.613 -10.542 20.102 1.00 17.01 ATOM 6631 O LEU 985 -8.613 -10.542 20.102 1.00 17.01 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 12.15 ATOM 6633 CD PRO 986 -7.280 -12.891 23.695 1.00 10.32 ATOM 6634 CA PRO 986 -7.280 -12.891 23.695 1.00 11.35 ATOM 6635 CB PRO 986 -7.238 -14.221 25.633 1.00 12.21 ATOM 6636 CG PRO 986 -9.309 -13.046 25.372 1.00 11.35 ATOM 6637 C PRO 986 -9.309 -13.046 26.482 1.00 10.32 ATOM 6639 N PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6640 CA PHE 987 -9.913 -12.938 28.856 1.00 10.31 ATOM 6640 CB PHE 987 -9.524 -13.722 30.118 1.00 10.32 ATOM 6640 CB PHE 987 -9.524 -13.614 27.684 1.00 10.31 ATOM 6645 CE1 PHE 987 -9.700 -12.984 31.418 1.00 10.30 ATOM 6646 CC2 PHE 987 -9.700 -12.984 31.418 1.00 10.30 ATOM 6648 CD1 PHE 987 -9.700 -12.984 31.418 1.00 10.30 ATOM 6645 CE1 PHE 987 -9.700 -12.984 31.418 1.00 12.08 ATOM 6646 CC2 PHE 987 -9.700 -12.984 31.418 1.00 12.08 ATOM 6648 CD1 PHE 987 -9.700 -12.984 31.418 1.00 12.08 ATOM 6648 CD1 PHE 987 -9.700 -12.994 31.418 1.00 12.08 ATOM 6648 CD1 PHE 987 -9.700 -12.994 31.418 1.00 12.08 ATOM 6648 CD1 PHE 987 -9.700 -12.994 31.418 1.00 12.08 ATOM 6648 CD1 PHE 987 -9.700 -12.994 31.418 1.00 12.08 ATOM 6648 CD1 PHE 987 -9.700 -12.994 31.418 1.00 12.08 ATOM 6648 CD1 PHE 987 -9.700 -12.994 31.418 1.00 12.08 ATOM 6648 CD1 PHE 987 -9.700 -12.994 31.418 1.00 12.08 ATOM 6648 CD2 PHE 987 -9.700 -12.994 31.418 1.00 12.08 ATOM 6648 CD1 PHE 987 -9.700 -12.994 31.418 1.00 12.08 | | | | | | | | | |
| ATOM 6622 C ASP 984 -9.390 -14.627 20.592 1.00 10.62 ATOM 6623 O ASP 984 -8.161 -14.538 20.524 1.00 10.17 ATOM 6624 N LEU 985 -10.151 -13.688 21.137 1.00 10.79 ATOM 6625 CA LEU 985 -9.529 -12.587 21.864 1.00 11.87 ATOM 6626 CB LEU 985 -10.323 -11.295 21.763 1.00 12.83 ATOM 6627 CG LEU 985 -10.091 -10.510 20.479 1.00 14.09 ATOM 6628 CD1 LEU 985 -10.537 -9.065 20.695 1.00 16.64 ATOM 6629 CD2 LEU 985 -8.613 -10.542 20.102 1.00 17.01 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6631 O LEU 985 -10.840 -13.590 23.606 1.00 12.15 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 10.32 ATOM 6633 CD PRO 986 -8.651 -13.315 24.034 1.00 10.32 ATOM 6634 CA PRO 986 -8.698 -13.906 25.372 1.00 10.52 ATOM 6635 CB PRO 986 -7.280 -12.891 23.695 1.00 10.52 ATOM 6637 C PRO 986 -6.563 -13.023 25.015 1.00 12.21 ATOM 6638 O PRO 986 -9.309 -13.046 26.482 1.00 12.95 ATOM 6638 O PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6639 N PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6640 CA PHE 987 -9.524 -13.722 30.118 1.00 10.31 ATOM 6640 CB PHE 987 -9.524 -13.722 30.118 1.00 10.31 ATOM 6640 CB PHE 987 -9.524 -13.722 30.118 1.00 10.32 ATOM 6640 CB PHE 987 -9.524 -13.722 30.118 1.00 10.31 ATOM 6644 CD2 PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6645 CE1 PHE 987 -9.524 -13.614 27.684 1.00 10.31 ATOM 6646 CE2 PHE 987 -9.524 -13.614 27.684 1.00 10.31 ATOM 6647 CD PHE 987 -9.524 -13.722 30.118 1.00 10.31 ATOM 6648 CD PHE 987 -9.524 -13.614 27.684 1.00 10.31 ATOM 6647 CD PHE 987 -9.524 -13.614 27.684 1.00 10.31 ATOM 6648 CD PHE 987 -9.524 -13.614 27.684 1.00 10.31 ATOM 6648 CD PHE 987 -9.524 -13.697 32.265 1.00 11.62 ATOM 6648 CD PHE 987 -9.524 -13.491 28.955 1.00 11.22 ATOM 6648 C PHE 987 -8.705 -12.697 33.493 1.00 12.09 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 13.84 ATOM 6649 O PHE 987 -9.421 -11.491 28.955 1.00 13.88 | | | | | | | | | |
| ATOM 6623 O ASP 984 -8.161 -14.538 20.524 1.00 10.17 ATOM 6624 N LEU 985 -10.151 -13.688 21.137 1.00 10.79 ATOM 6625 CA LEU 985 -9.529 -12.587 21.864 1.00 11.87 ATOM 6626 CB LEU 985 -10.323 -11.295 21.763 1.00 12.83 ATOM 6627 CG LEU 985 -10.091 -10.510 20.479 1.00 14.09 ATOM 6628 CD1 LEU 985 -10.537 -9.065 20.695 1.00 14.09 ATOM 6630 C LEU 985 -8.613 -10.542 20.102 1.00 17.01 ATOM 6631 O LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 10.32 ATOM 6633 CD PRO 986 -8.651 -13.315 24.034 1.00 10.32 ATOM 6634 CA PRO 986 -8.698 -13.906 25.372 1.00 10.52 ATOM 6635 CB PRO 986 -6.563 -13.023 25.015 1.00 12.215 ATOM 6636 CG PRO 986 -6.563 -13.023 25.015 1.00 12.25 ATOM 6638 O PRO 986 -6.563 -13.023 25.015 1.00 12.75 ATOM 6638 O PRO 986 -9.309 -13.046 26.482 1.00 10.93 ATOM 6639 N PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6640 CA PHE 987 -9.524 -13.722 30.118 1.00 10.31 ATOM 6640 CB PHE 987 -9.524 -13.722 30.118 1.00 11.93 ATOM 6640 CB PHE 987 -9.524 -13.722 30.118 1.00 11.95 ATOM 6645 CE1 PHE 987 -9.770 -12.984 31.418 1.00 10.30 ATOM 6645 CE1 PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6646 CE2 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6648 C PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6648 C PHE 987 -8.705 -12.697 32.265 1.00 13.41 ATOM 6648 C PHE 987 -9.9421 -11.294 28.955 1.00 13.41 ATOM 6648 C PHE 987 -9.9421 -11.491 28.955 1.00 13.41 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 13.41 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 13.41 | | | | | | | | | |
| ATOM 6624 N LEU 985 -10.151 -13.688 21.137 1.00 10.79 ATOM 6625 CA LEU 985 -9.529 -12.587 21.864 1.00 11.87 ATOM 6626 CB LEU 985 -10.323 -11.295 21.763 1.00 12.83 ATOM 6627 CG LEU 985 -10.091 -10.510 20.479 1.00 14.09 ATOM 6628 CD1 LEU 985 -10.537 -9.065 20.695 1.00 16.64 ATOM 6629 CD2 LEU 985 -8.613 -10.542 20.102 1.00 17.01 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6631 O LEU 985 -10.840 -13.590 23.606 1.00 12.15 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 10.32 ATOM 6633 CD PRO 986 -7.280 -12.891 23.695 1.00 10.52 ATOM 6634 CA PRO 986 -8.698 -13.906 25.372 1.00 10.52 ATOM 6636 CG PRO 986 -6.563 -13.023 25.015 1.00 12.21 ATOM 6637 C PRO 986 -6.563 -13.023 25.015 1.00 12.21 ATOM 6638 O PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6639 N PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6640 CA PHE 987 -9.913 -12.938 28.856 1.00 10.31 ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6642 CG PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6644 CD2 PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6644 CD2 PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6645 CE1 PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6646 CE2 PHE 987 -9.770 -12.984 31.418 1.00 12.08 ATOM 6648 C PHE 987 -8.705 -12.697 32.265 1.00 13.41 ATOM 6648 C PHE 987 -8.705 -12.697 33.885 1.00 13.418 ATOM 6648 C PHE 987 -9.770 -12.984 31.418 1.00 13.418 ATOM 6648 C PHE 987 -9.770 -12.984 31.418 1.00 13.418 ATOM 6648 C PHE 987 -9.770 -12.984 31.418 1.00 12.08 ATOM 6648 C PHE 987 -9.770 -12.984 31.418 1.00 13.418 ATOM 6648 C PHE 987 -9.770 -12.984 31.418 1.00 13.418 ATOM 6648 C PHE 987 -9.770 -12.984 31.418 1.00 13.418 ATOM 6648 C PHE 987 -9.770 -12.984 31.418 1.00 13.418 ATOM 6648 C PHE 987 -9.770 -12.984 31.418 1.00 13.418 ATOM 6648 C PHE 987 -9.770 -12.984 31.418 1.00 13.418 | | | | | | | | | |
| ATOM 6625 CA LEU 985 | | | 0 | | | | | | |
| ATOM 6626 CB LEU 985 -10.323 -11.295 21.763 1.00 12.83 ATOM 6627 CG LEU 985 -10.091 -10.510 20.479 1.00 14.09 ATOM 6628 CD1 LEU 985 -10.537 -9.065 20.695 1.00 16.64 ATOM 6629 CD2 LEU 985 -8.613 -10.542 20.102 1.00 17.01 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6631 O LEU 985 -10.840 -13.590 23.606 1.00 12.15 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 10.32 ATOM 6633 CD PRO 986 -7.280 -12.891 23.695 1.00 10.52 ATOM 6634 CA PRO 986 -8.698 -13.906 25.372 1.00 11.35 ATOM 6635 CB PRO 986 -7.238 -14.221 25.633 1.00 12.21 ATOM 6636 CG PRO 986 -6.563 -13.023 25.015 1.00 12.21 ATOM 6637 C PRO 986 -6.563 -13.023 25.015 1.00 12.75 ATOM 6638 O PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6639 N PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6640 CA PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6641 CB PHE 987 -9.913 -12.938 28.856 1.00 10.31 ATOM 6642 CG PHE 987 -9.770 -12.938 28.856 1.00 10.31 ATOM 6643 CD1 PHE 987 -9.770 -12.944 31.418 1.00 11.95 ATOM 6644 CD2 PHE 987 -9.770 -12.944 31.418 1.00 11.95 ATOM 6645 CE1 PHE 987 -9.770 -12.944 31.418 1.00 12.08 ATOM 6646 CE2 PHE 987 -8.705 -12.697 32.265 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.705 -12.697 33.493 1.00 12.08 ATOM 6648 C PHE 987 -8.910 -12.774 33.885 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 13.88 | MOTA | 6624 | N | LEU | 985 | -10.151 | -13.688 | 21.137 | 1.00 10.79 |
| ATOM 6627 CG LEU 985 -10.091 -10.510 20.479 1.00 14.09 ATOM 6628 CD1 LEU 985 -10.537 -9.065 20.695 1.00 16.64 ATOM 6629 CD2 LEU 985 -8.613 -10.542 20.102 1.00 17.01 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6631 O LEU 985 -10.840 -13.590 23.606 1.00 12.15 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 10.32 ATOM 6633 CD PRO 986 -7.280 -12.891 23.695 1.00 10.52 ATOM 6634 CA PRO 986 -8.698 -13.906 25.372 1.00 11.35 ATOM 6635 CB PRO 986 -7.238 -14.221 25.633 1.00 12.21 ATOM 6636 CG PRO 986 -6.563 -13.023 25.015 1.00 12.21 ATOM 6637 C PRO 986 -9.309 -13.023 25.015 1.00 12.75 ATOM 6638 O PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6639 N PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6640 CA PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 10.31 ATOM 6642 CG PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6643 CD1 PHE 987 -9.524 -13.728 31.418 1.00 10.30 ATOM 6644 CD2 PHE 987 -9.770 -12.984 31.418 1.00 10.30 ATOM 6645 CE1 PHE 987 -8.705 -12.697 32.265 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.705 -12.697 33.493 1.00 12.08 ATOM 6647 CZ PHE 987 -8.705 -12.697 33.493 1.00 12.08 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 13.88 | MOTA | 6625 | CA | LEU | 985 | -9.529 | -12.587 | 21.864 | 1.00 11.87 |
| ATOM 6628 CD1 LEU 985 -10.537 -9.065 20.695 1.00 16.64 ATOM 6629 CD2 LEU 985 -8.613 -10.542 20.102 1.00 17.01 ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6631 O LEU 985 -10.840 -13.590 23.606 1.00 12.15 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 10.32 ATOM 6633 CD PRO 986 -7.280 -12.891 23.695 1.00 10.52 ATOM 6635 CB PRO 986 -8.698 -13.906 25.372 1.00 11.35 ATOM 6635 CB PRO 986 -7.238 -14.221 25.633 1.00 12.21 ATOM 6636 CG PRO 986 -6.563 -13.023 25.015 1.00 12.75 ATOM 6637 C PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6638 O PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6639 N PHE 987 -9.364 -13.913 22.255 1.00 10.33 ATOM 6640 CA PHE 987 -9.913 -12.938 28.856 1.00 10.31 ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 12.08 ATOM 6642 CG PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6644 CD2 PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6645 CE1 PHE 987 -8.705 -12.697 32.265 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.705 -12.697 32.265 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.705 -12.697 32.265 1.00 13.41 ATOM 6647 CZ PHE 987 -8.910 -12.770 33.493 1.00 12.09 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -9.421 -11.491 28.955 1.00 11.22 | ATOM | 6626 | CB | LEU | 985 | -10.323 | -11.295 | 21.763 | 1.00 12.83 |
| ATOM 6630 C LEU 985 | ATOM | 6627 | CG | LEU | 985 | -10.091 | -10.510 | | 1.00 14.09 |
| ATOM 6630 C LEU 985 | ATOM | 6628 | CD1 | LEU | 985 | -10.537 | -9.065 | 20.695 | 1.00 16.64 |
| ATOM 6630 C LEU 985 -9.725 -13.204 23.247 1.00 11.19 ATOM 6631 O LEU 985 -10.840 -13.590 23.606 1.00 12.15 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 10.32 ATOM 6633 CD PRO 986 -7.280 -12.891 23.695 1.00 10.52 ATOM 6634 CA PRO 986 -8.698 -13.906 25.372 1.00 11.35 ATOM 6635 CB PRO 986 -7.238 -14.221 25.633 1.00 12.21 ATOM 6636 CG PRO 986 -6.563 -13.023 25.015 1.00 12.75 ATOM 6637 C PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6638 O PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6639 N PHE 987 -9.364 -12.938 28.856 1.00 10.31 ATOM 6640 CA PHE 987 -9.913 -12.938 28.856 1.00 10.31 ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6642 CG PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6644 CD2 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6645 CE1 PHE 987 -8.705 -12.697 32.265 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.705 -12.697 33.493 1.00 12.08 ATOM 6647 CZ PHE 987 -8.910 -12.700 33.493 1.00 12.09 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -9.421 -11.491 28.955 1.00 11.22 | | | | | | | | | |
| ATOM 6631 O LEU 985 -10.840 -13.590 23.606 1.00 12.15 ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 10.32 ATOM 6633 CD PRO 986 -7.280 -12.891 23.695 1.00 10.52 ATOM 6634 CA PRO 986 -8.698 -13.906 25.372 1.00 11.35 ATOM 6635 CB PRO 986 -7.238 -14.221 25.633 1.00 12.21 ATOM 6636 CG PRO 986 -6.563 -13.023 25.015 1.00 12.75 ATOM 6637 C PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6638 O PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6639 N PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6640 CA PHE 987 -9.913 -12.938 28.856 1.00 10.31 ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6642 CG PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6644 CD2 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6645 CE1 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6646 CE2 PHE 987 -8.705 -12.697 33.493 1.00 12.08 ATOM 6647 CZ PHE 987 -8.910 -12.770 33.493 1.00 12.09 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -9.421 -11.491 28.955 1.00 11.22 | | | | | | | | | |
| ATOM 6632 N PRO 986 -8.651 -13.315 24.034 1.00 10.32 ATOM 6633 CD PRO 986 -7.280 -12.891 23.695 1.00 10.52 ATOM 6634 CA PRO 986 -8.698 -13.906 25.372 1.00 11.35 ATOM 6635 CB PRO 986 -7.238 -14.221 25.633 1.00 12.21 ATOM 6636 CG PRO 986 -6.563 -13.023 25.015 1.00 12.75 ATOM 6637 C PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6638 O PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6639 N PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6640 CA PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6641 CB PHE 987 -9.524 -13.2938 28.856 1.00 10.31 ATOM 6642 CG PHE 987 -9.770 -12.938 28.856 1.00 10.30 ATOM 6643 CD1 PHE 987 -9.770 -12.948 31.418 1.00 11.95 ATOM 6644 CD2 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6645 CE1 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6646 CE2 PHE 987 -8.705 -12.697 33.493 1.00 12.09 ATOM 6647 CZ PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -9.421 -11.491 28.955 1.00 11.22 | | | | | | | | | |
| ATOM 6633 CD PRO 986 -7.280 -12.891 23.695 1.00 10.52 ATOM 6634 CA PRO 986 -8.698 -13.906 25.372 1.00 11.35 ATOM 6635 CB PRO 986 -7.238 -14.221 25.633 1.00 12.21 ATOM 6636 CG PRO 986 -6.563 -13.023 25.015 1.00 12.75 ATOM 6637 C PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6638 O PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6639 N PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6640 CA PHE 987 -9.913 -12.938 28.856 1.00 10.31 ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6642 CG PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6644 CD2 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6646 CE2 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6646 CE2 PHE 987 -8.910 -12.707 33.493 1.00 12.09 ATOM 6647 CZ PHE 987 -8.910 -12.707 33.493 1.00 12.09 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -8.223 -11.220 28.861 1.00 9.94 | | | | | | | | | |
| ATOM 6634 CA PRO 986 -8.698 -13.906 25.372 1.00 11.35 ATOM 6635 CB PRO 986 -7.238 -14.221 25.633 1.00 12.21 ATOM 6636 CG PRO 986 -6.563 -13.023 25.015 1.00 12.75 ATOM 6637 C PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6638 O PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6639 N PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6640 CA PHE 987 -9.913 -12.938 28.856 1.00 10.31 ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6642 CG PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6643 CD1 PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6644 CD2 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6645 CE1 PHE 987 -8.705 -12.697 32.265 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.910 -12.703 33.493 1.00 12.09 ATOM 6647 CZ PHE 987 -8.910 -12.704 33.885 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -8.223 -11.220 28.861 1.00 9.94 | | | | | | | | | |
| ATOM 6635 CB PRO 986 -7.238 -14.221 25.633 1.00 12.21 ATOM 6636 CG PRO 986 -6.563 -13.023 25.015 1.00 12.75 ATOM 6637 C PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6638 O PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6639 N PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6640 CA PHE 987 -9.913 -12.938 28.856 1.00 10.31 ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6642 CG PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6643 CD1 PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6644 CD2 PHE 987 -8.705 -12.630 31.821 1.00 12.08 ATOM 6645 CE1 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6646 CE2 PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6647 CZ PHE 987 -8.910 -12.703 33.493 1.00 12.09 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -9.421 -11.491 28.955 1.00 11.22 | | | - | | | | | | |
| ATOM 6636 CG PRO 986 -6.563 -13.023 25.015 1.00 12.75 ATOM 6637 C PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6638 O PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6639 N PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6640 CA PHE 987 -9.913 -12.938 28.856 1.00 10.31 ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6642 CG PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6643 CD1 PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6644 CD2 PHE 987 -8.705 -12.630 31.821 1.00 12.08 ATOM 6645 CE1 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6646 CE2 PHE 987 -8.910 -12.999 33.054 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.910 -12.700 33.493 1.00 12.09 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -9.421 -11.491 28.955 1.00 11.22 | | | | | | | | | |
| ATOM 6637 C PRO 986 -9.309 -13.046 26.482 1.00 10.95 ATOM 6638 O PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6639 N PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6640 CA PHE 987 -9.913 -12.938 28.856 1.00 10.31 ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6642 CG PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6643 CD1 PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6644 CD2 PHE 987 -8.705 -12.630 31.821 1.00 12.08 ATOM 6645 CE1 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6646 CE2 PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6647 CZ PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -8.223 -11.220 28.861 1.00 9.94 | | | | | | | | | |
| ATOM 6638 O PRO 986 -9.721 -11.914 26.255 1.00 10.33 ATOM 6639 N PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6640 CA PHE 987 -9.913 -12.938 28.856 1.00 10.31 ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 10.31 ATOM 6642 CG PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6643 CD1 PHE 987 -9.770 -12.630 31.821 1.00 12.08 ATOM 6644 CD2 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6645 CE1 PHE 987 -11.272 -11.999 33.054 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6647 CZ PHE 987 -10.196 -11.724 33.885 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -8.223 -11.220 28.861 1.00 9.94 | MOTA | 6636 | CG | PRO | 986 | | | | |
| ATOM 6649 N PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6640 CA PHE 987 -9.913 -12.938 28.856 1.00 10.31 ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6642 CG PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6643 CD1 PHE 987 -11.054 -12.630 31.821 1.00 12.08 ATOM 6644 CD2 PHE 987 -8.705 -12.630 31.821 1.00 11.62 ATOM 6645 CE1 PHE 987 -11.272 -11.999 33.054 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6647 CZ PHE 987 -10.196 -11.724 33.885 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -8.223 -11.220 28.861 1.00 9.94 | ATOM | | C | PRO | 986 | | | | |
| ATOM 6649 N PHE 987 -9.364 -13.614 27.684 1.00 9.49 ATOM 6640 CA PHE 987 -9.913 -12.938 28.856 1.00 10.31 ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6642 CG PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6643 CD1 PHE 987 -11.054 -12.630 31.821 1.00 12.08 ATOM 6644 CD2 PHE 987 -8.705 -12.630 31.821 1.00 11.62 ATOM 6645 CE1 PHE 987 -11.272 -11.999 33.054 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6647 CZ PHE 987 -10.196 -11.724 33.885 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -8.223 -11.220 28.861 1.00 9.94 | ATOM | 6638 | 0 | PRO | 986 | -9.721 | -11.914 | 26.255 | 1.00 10.33 |
| ATOM 6640 CA PHE 987 -9.913 -12.938 28.856 1.00 10.31 ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6642 CG PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6643 CD1 PHE 987 -11.054 -12.630 31.821 1.00 12.08 ATOM 6644 CD2 PHE 987 -8.705 -11.697 32.265 1.00 11.62 ATOM 6645 CE1 PHE 987 -11.272 -11.999 33.054 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6647 CZ PHE 987 -10.196 -11.724 33.885 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -8.223 -11.220 28.861 1.00 9.94 | | | N | | 987 | -9.364 | -13.614 | 27.684 | 1.00 9.49 |
| ATOM 6641 CB PHE 987 -9.524 -13.722 30.118 1.00 10.30 ATOM 6642 CG PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6643 CD1 PHE 987 -11.054 -12.630 31.821 1.00 12.08 ATOM 6644 CD2 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6645 CE1 PHE 987 -11.272 -11.999 33.054 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6647 CZ PHE 987 -10.196 -11.724 33.885 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -8.223 -11.220 28.861 1.00 9.94 | | | | | | | | 28.856 | |
| ATOM 6642 CG PHE 987 -9.770 -12.984 31.418 1.00 11.95 ATOM 6643 CD1 PHE 987 -11.054 -12.630 31.821 1.00 12.08 ATOM 6644 CD2 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6645 CE1 PHE 987 -11.272 -11.999 33.054 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6647 CZ PHE 987 -10.196 -11.772 33.885 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -8.223 -11.220 28.861 1.00 9.94 | | | | | | | | | |
| ATOM 6643 CD1 PHE 987 -11.054 -12.630 31.821 1.00 12.08 ATOM 6644 CD2 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6645 CE1 PHE 987 -11.272 -11.999 33.054 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6647 CZ PHE 987 -10.196 -11.724 33.885 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -8.223 -11.220 28.861 1.00 9.94 | | | | | | | | | |
| ATOM 6644 CD2 PHE 987 -8.705 -12.697 32.265 1.00 11.62 ATOM 6645 CE1 PHE 987 -11.272 -11.999 33.054 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6647 CZ PHE 987 -10.196 -11.724 33.885 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -8.223 -11.220 28.861 1.00 9.94 | | | | | | | | | |
| ATOM 6645 CE1 PHE 987 -11.272 -11.999 33.054 1.00 13.41 ATOM 6646 CE2 PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6647 CZ PHE 987 -10.196 -11.724 33.885 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -8.223 -11.220 28.861 1.00 9.94 | | | | | | | | | |
| ATOM 6646 CE2 PHE 987 -8.910 -12.070 33.493 1.00 12.09 ATOM 6647 CZ PHE 987 -10.196 -11.724 33.885 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -8.223 -11.220 28.861 1.00 9.94 | | | | | | | | | |
| ATOM 6647 CZ PHE 987 -10.196 -11.724 33.885 1.00 13.88 ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -8.223 -11.220 28.861 1.00 9.94 | | | | | | | | | |
| ATOM 6648 C PHE 987 -9.421 -11.491 28.955 1.00 11.22 ATOM 6649 O PHE 987 -8.223 -11.220 28.861 1.00 9.94 | | | | | | | | | |
| ATOM 6649 O PHE 987 -8.223 -11.220 28.861 1.00 9.94 | | | | | | | | | |
| | | | С | PHE | | | | | |
| | ATOM | 6649 | 0 | PHE | 987 | | | | |
| | MOTA | | N | | 988 | -10.371 | -10.579 | 29.136 | 1.00 10.88 |

| MOTA | 6651 | CA | MET | 988 | -10.118 | -9.153 | 29.274 | 1.00 12.00 |
|------|-------|-----|-----|-----|---------|------------------|--------|------------|
| ATOM | 6652 | CB | MET | 988 | -9.447 | -8.854 | 30.630 | 1.00 11.75 |
| ATOM | 6653 | CG | MET | 988 | -9.721 | -7.436 | 31.166 | 1.00 13.31 |
| ATOM | 6654 | SD | MET | 988 | -11.475 | -7.116 | 31.566 | 1.00 13.55 |
| ATOM | 6655 | CE | MET | 988 | -11.538 | -7.686 | 33.263 | 1.00 18.85 |
| ATOM | 6656 | C | MET | 988 | -9.300 | -8.512 | 28.159 | 1.00 13.38 |
| | | | | 988 | -8.568 | -7.556 | 28.411 | 1.00 15.30 |
| ATOM | 6657 | 0 | MET | | | | | |
| ATOM | 6658 | N | ALA | 989 | -9.420 | -9.019 | 26.937 | 1.00 11.97 |
| MOTA | 6659 | CA | ALA | 989 | -8.681 | -8.450 | 25.816 | 1.00 12.87 |
| MOTA | 6660 | CB | ALA | 989 | -8.073 | -9.568 | 24.953 | 1.00 11.39 |
| ATOM | 6661 | С | ALA | 989 | -9.585 | -7.554 | 24.959 | 1.00 12.13 |
| MOTA | 6662 | Ο. | ALA | 989 | -9.158 | -7.019 | 23.938 | 1.00 14.24 |
| MOTA | 6663 | N | TYR | 990 | -10.833 | -7.391 | 25.389 | 1.00 11.11 |
| MOTA | 6664 | CA | TYR | 990 | -11.786 | -6.538 | 24.694 | 1.00 11.34 |
| ATOM | 6665 | CB | TYR | 990 | -12.591 | -7.352 | 23.660 | 1.00 11.56 |
| ATOM | 6666 | CG | TYR | 990 | -13.140 | -8.668 | 24.180 | 1.00 14.52 |
| ATOM | 6667 | CD1 | TYR | 990 | -14.464 | -8.776 | 24.593 | 1.00 11.96 |
| ATOM | 6668 | CE1 | TYR | 990 | -14.979 | -9.979 | 25.082 | 1.00 14.62 |
| ATOM | .6669 | CD2 | TYR | 990 | -12.327 | -9.802 | 24.267 | 1.00 12.94 |
| ATOM | 6670 | CE2 | TYR | 990 | -12.825 | -11.017 | 24.759 | 1.00 14.62 |
| ATOM | 6671 | CZ | TYR | 990 | -14.156 | -11.091 | 25.163 | 1.00 15.49 |
| ATOM | 6672 | ОН | TYR | 990 | -14.675 | -12.270 | 25.655 | 1.00 18.21 |
| ATOM | 6673 | C | TYR | 990 | -12.706 | -5.851 | 25.711 | 1.00 12.49 |
| ATOM | 6674 | ō | TYR | 990 | -13.906 | -5.689 | 25.481 | 1.00 14.32 |
| | 6675 | N | ALA | 991 | -12.116 | -5.430 | 26.827 | 1.00 14.32 |
| ATOM | 6676 | | | | -12.844 | -4.770 | 27.913 | 1.00 12.75 |
| MOTA | | CA | ALA | 991 | | | 29.104 | |
| ATOM | 6677 | CB | ALA | 991 | -11.927 | -4.561 | | 1.00 11.96 |
| MOTA | 6678 | С | ALA | 991 | -13.424 | -3.434 | 27.478 | 1.00 12.37 |
| MOTA | 6679 | 0 | ALA | 991 | -14.410 | -2.963 | 28.044 | 1.00 12.98 |
| MOTA | 6680 | N | THR | 992 | -12.779 | -2.803 | 26.505 | 1.00 13.27 |
| MOTA | 6681 | CA | THR | 992 | -13.248 | -1.527 | 25.967 | 1.00 13.52 |
| ATOM | 6682 | CB | THR | 992 | -12.390 | -0.333 | 26.462 | 1.00 15.27 |
| MOTA | 6683 | OG1 | THR | 992 | -11.069 | -0.437 | 25.918 | 1.00 15.35 |
| MOTA | 6684 | CG2 | THR | 992 | -12.286 | -0.326 | 27.983 | 1.00 15.49 |
| MOTA | 6685 | С | THR | 992 | -13.093 | -1.640 | 24.454 | 1.00 15.81 |
| MOTA | 6686 | Ο. | THR | 992 | -12.316 | -2.463 | 23.965 | 1.00 11.88 |
| MOTA | 6687 | N | PRO | 993 | -13.849 | -0.839 | 23.690 | 1.00 14.26 |
| MOTA | 6688 | CD | PRO | 993 | -15.022 | -0.033 | 24.082 | 1.00 14.65 |
| ATOM | 6689 | CA | PRO | 993 | -13.723 | -0.912 | 22.233 | 1.00 15.27 |
| ATOM | 6690 | CB | PRO | 993 | -14.663 | 0.189 | 21.756 | 1.00 13.69 |
| ATOM | 6691 | CG | PRO | 993 | -15.781 | 0.103 | 22.771 | 1.00 14.48 |
| ATOM | 6692 | С | PRO | 993 | -12.279 | -0.675 | 21.794 | 1.00 15.17 |
| ATOM | 6693 | ō | PRO | 993 | -11.745 | -1.403 | 20.955 | 1.00 14.48 |
| ATOM | 6694 | N | GLU | 994 | -11.656 | 0.343 | 22.383 | 1.00 14.90 |
| ATOM | 6695 | CA | GLU | 994 | -10.284 | 0.714 | 22.068 | 1.00 16.61 |
| ATOM | 6696 | CB | GLU | 994 | -9.847 | 1.881 | 22.951 | 1.00 20.94 |
| ATOM | 6697 | CG | GLU | 994 | -8.673 | 2.652 | 22.415 | 1.00 29.96 |
| ATOM | 6698 | CD | GLU | 994 | -8.335 | 3.857 | 23.277 | 1.00 23.30 |
| ATOM | | OE1 | | 994 | -7.498 | 3.719 | 24.199 | 1.00 35.55 |
| | 6699 | | | | | 4.934 | 23.038 | |
| MOTA | 6700 | OE2 | GLU | 994 | -8.923 | | | |
| ATOM | 6701 | C | GLU | 994 | -9.313 | -0.447 | 22.256 | 1.00 15.95 |
| MOTA | 6702 | 0 | GLU | 994 | -8.439 | -0.675 | 21.421 | 1.00 14.70 |
| ATOM | 6703 | N | GLN | 995 | -9.455 | -1.170 | 23.361 | 1.00 14.74 |
| ATOM | 6704 | CA | GLN | 995 | -8.586 | -2.307 | 23.625 | 1.00 14.57 |
| MOTA | 6705 | CB | GLN | 995 | -8.758 | -2.793 | 25.058 | 1.00 15.85 |
| MOTA | 6706 | CG | GLN | 995 | -8.325 | -1.765 | 26.084 | 1.00 22.47 |
| MOTA | 6707 | CD | GLN | 995 | -8.360 | -2.315 | 27.480 | 1.00 26.05 |
| MOTA | 6708 | OE1 | | 995 | -7.468 | -3.057 | 27.886 | 1.00 27.48 |
| MOTA | 6709 | NE2 | GLN | 995 | -9.414 | -1.980 | 28.225 | 1.00 29.12 |
| MOTA | 6710 | С | GLN | 995 | -8.892 | -3.433 | 22.664 | 1.00 11.23 |
| MOTA | 6711 | 0 | GLN | 995 | -7.992 | -4.142 | 22.222 | 1.00 12.90 |
| ATOM | 6712 | N | ALA | 996 | -10.170 | -3.612 | 22.361 | 1.00 11.62 |
| MOTA | 6713 | CA | ALA | 996 | -10.578 | -4.647 | 21.422 | 1.00 10.29 |
| ATOM | 6714 | CB | ALA | 996 | -12.103 | -4.647 | 21.266 | 1.00 12.23 |
| MOTA | 6715 | С | ALA | 996 | -9.917 | -4.396 | 20.069 | 1.00 11.82 |
| MOTA | 6716 | Ō | ALA | 996 | -9.402 | -5.321 | 19.431 | 1.00 11.66 |
| ATOM | 6717 | N | PHE | 997 | -9.933 | -3.141 | 19.621 | 1.00 11.85 |
| MOTA | 6718 | CA | PHE | 997 | -9.325 | -2.808 | 18.327 | 1.00 13.01 |
| ATOM | 6719 | СВ | PHE | 997 | -9.423 | -1.308 | 18.025 | 1.00 12.43 |
| ATOM | 6720 | CG | PHE | 997 | -10.813 | -0.747 | 18.100 | 1.00 12.02 |
| ATOM | 6721 | | PHE | 997 | -11.921 | -1.528 | 17.811 | 1.00 14.72 |
| ATOM | 6722 | | PHE | 997 | -11.001 | 0.588 | 18.443 | 1.00 15.95 |
| ATOM | 6723 | | PHE | 997 | -13.209 | -0.992 | 17.865 | 1.00 15.33 |
| ATOM | | | | 997 | -12.279 | 1.140 | 18.499 | 1.00 10.49 |
| | 6724 | | PHE | | | | 18.499 | 1.00 13.96 |
| ATOM | 6725 | CZ | PHE | 997 | -13.379 | 0.344 -3.179 | 18.211 | 1.00 17.62 |
| ATOM | 6726 | C | PHE | 997 | -7.846 | -3.179 -3.784 | | 1.00 13.37 |
| MOTA | 6727 | 0 | PHE | 997 | -7.364 | -3.704 | 17.343 | 1.00 13.24 |

| ATOM | 6728 | N | GLU | 998 | | -7.128 | -2.779 | 19.341 | 1.00 13.15 |
|--------------|--------------|--------|------------|--------------|----|------------------|--------------------|------------------|--------------------------|
| ATOM | 6729 | CA | GLU | 998 | | -5.701 | -3.054 | 19.430 | 1.00 15.16 |
| ATOM | 6730 | CB | GLU | 998 | | -5.123 | -2.380 | 20.674 | 1.00 17.72 |
| ATOM | 6731 | CG | GLU | 998 | | -3.669 | -2.700 | 20.952 | 1.00 24.55 |
| ATOM | 6732 | CD | GLU | 998 | | -2.709 | -1.972 | 20.023 | 1.00 28.59 |
| MOTA | 6733 | OE1 | GLU | 998 | | -3.168 | -1.301 | 19.068 | 1.00 30.41 |
| ATOM | 6734 | OE2 | | 998 | | -1.486 | -2.077 | 20.254 | 1.00 31.76 |
| MOTA | 6735 | С | GLU | 998 | | -5.389 | -4.554 | 19.461 | 1.00 12.56 |
| ATOM | 6736 | 0 | GLU | 998 | | -4.523 | -5.029 | 18.730 | 1.00 10.73 |
| ATOM | 6737 | N | ASN | 999 | | -6.093 | -5.303 | 20.301 | 1.00 12.22 |
| ATOM | 6738 | CA | ASN | 999 | | -5.833 | -6.729 | 20.393 | 1.00 12.09 |
| ATOM | 6739 | CB | ASN | 999 | | -6.429 | -7.280 | 21.694 | 1.00 11.99 |
| ATOM | 6740 | CG | ASN | 999 | | -5.719 | -6.735 | 22.912 | 1.00 14.10 |
| MOTA | 6741 | | ASN | 999 | | -4.503 | -6.514 | 22.869 | 1.00 13.95 1.00 13.68 |
| ATOM | 6742 | | ASN | 999 | | -6.456 -6.304 | -6.520 -7.523 | 24.010 19.182 | 1.00 13.68 |
| ATOM | 6743 6744 | С 0 | ASN ASN | 999 999 | | -5.667 | -8.504 | 18.775 | 1.00 12.22 |
| ATOM ATOM | 6745 | N | ALA | 1000 | | -7.411 | -7.101 | 18.589 | 1.00 10.24 |
| ATOM | 6746 | CA | ALA | 1000 | | -7.912 | -7.777 | 17.399 | 1.00 12.27 |
| ATOM | 6747 | CB | ALA | 1000 | | -9.280 | -7.201 | 16.998 | 1.00 11.29 |
| ATOM | 6748 | C | ALA | 1000 | | -6.894 | -7.571 | 16.265 | 1.00 12.84 |
| ATOM | 6749 | ō | ALA | 1000 | | -6.617 | -8.488 | 15.493 | 1.00 11.51 |
| ATOM | 6750 | N | ALA | 1001 | | -6.325 | -6.371 | 16.174 | 1.00 12.62 |
| ATOM | 6751 | CA | ALA | 1001 | | -5.340 | -6.094 | 15.128 | 1.00 12.98 |
| ATOM | 6752 | СВ | ALA | 1001 | | -4.941 | -4.619 | 15.165 | 1.00 11.69 |
| ATOM | 6753 | С | ALA | 1001 | | -4.107 | -6.978 | 15.300 | 1.00 11.52 |
| MOTA | 6754 | 0 | ALA | 1001 | | -3.545 | -7.477 | 14.324 | 1.00 11.98 |
| MOTA | 6755 | N | THR | 1002 | - | -3.681 | -7.165 | 16.542 | 1.00 10.66 |
| MOTA | 6756 | CA | THR | 1002 | | -2.515 | -8.007 | 16.804 | 1.00 11.02 |
| MOTA | 6757 | CB | THR | 1002 | | -2.228 | -8.117 | 18.319 | 1.00 11.27 |
| ATOM | 6758 | OG1 | THR | 1002 | | -1.930 | -6.813 | 18.841 | 1.00 12.88 |
| MOTA | 6759 | CG2 | THR | 1002 | ٠. | -1.036 | -9.040 | 18.584 | 1.00 11.56 |
| ATOM | 6760 | С | THR | 1002 | | -2.739 | -9.411 | 16.246 | 1.00 10.94 |
| ATOM | 6761 | 0 | THR | 1002 | | -1.897 | -9.952 | 15.523 | 1.00 11.20 |
| ATOM | 6762 | N | VAL | 1003 | | | -10.005 | 16.563 | 1.00 9.24 |
| ATOM | 6763 | CA | VAL | 1003 | | | -11.372 | 16.102 | 1.00 9.83 |
| ATOM | 6764 | CB | VAL | 1003 | | | -11.991 | 16.897 | 1.00 11.74 |
| ATOM | 6765 | | VAL | 1003 | | | -11.511 | 16.373 | 1.00 10.79 |
| ATOM | 6766 | | VAL | 1003 | | | -13.484 | 16.875 | 1.00 19.69 |
| ATOM | 6767 | С | VAL | 1003 | | | -11.466 -12.462 | 14.593 13.965 | 1.00 10.01 1.00 7.78 |
| ATOM ATOM | 6768 6769 | O N | VAL MET | 1003 1004 | | | -12.402 | 14.013 | 1.00 7.78 |
| ATOM | 6770 | CA | MET | 1004 | | | -10.368 | 12.570 | 1.00 11.82 |
| ATOM | 6771 | CB | MET | 1004 | | -6.107 | -9.174 | 12.213 | 1.00 11.14 |
| ATOM | 6772 | CG | MET | 1004 | | -7.523 | -9.240 | 12.728 | 1.00 16.34 |
| ATOM | 6773 | SD | MET | 1004 | | | -10.464 | 11.934 | 1.00 19.40 |
| ATOM | 6774 | CE | MET | 1004 | | -8.653 | -9.772 | 10.242 | 1.00 17.67 |
| ATOM | 6775 | C | MET | 1004 | | | -10.211 | 11.825 | 1.00 10.89 |
| ATOM | 6776 | 0 | MET | 1004 | | -3.665 | -10.860 | 10.807 | 1.00 13.67 |
| ATOM | 6777 | N | ARG | 1005 | | -2.988 | -9.345 | 12.311 | 1.00 11.14 |
| ATOM | 6778 | CA | ARG | 1005 | | -1.708 | -9.184 | 11.619 | 1.00 11.02 |
| ATOM | 6779 | CB | ARG | 1005 | | -0.862 | -8.066 | 12.234 | 1.00 12.00 |
| ATOM | 6780 | CG | ARG | 1005 | | -1.490 | -6.689 | 12.114 | 1.00 16.37 |
| ATOM | 6781 | CD | ARG | 1005 | | -0.472 | -5.584 | 12.356 | 1.00 15.62 |
| ATOM | 6782 | NE | ARG | 1005 | | -1.134 | -4.292 | 12.558 | 1.00 17.19 |
| ATOM | 6783 | CZ | ARG | 1005 | | -1.491 | -3.811 | 13.744 | 1.00 16.30 |
| ATOM | 6784 | | ARG | 1005 | | -1.248 | -4.501 | 14.854 | 1.00 16.09 |
| MOTA | 6785 | | | -1005 | | -2.110 | -2.646 | 13.818 | 1.00 17.74 1.00 11.70 |
| ATOM | 6786 6787 | C | ARG ARG | 1005 1005 | | | -10.491 -10.787 | 11.659 10.750 | 1.00 11.70 1.00 11.26 |
| ATOM ATOM | 6788 | O N | ALA | 1005 | | | -11.266 | 12.716 | 1.00 11.20 |
| ATOM | 6789 | CA | ALA | 1006 | | | -12.540 | 12.710 | 1.00 11.42 |
| ATOM | 6790 | CB | ALA | 1006 | | | -12.996 | 14.363 | 1.00 12.29 |
| ATOM | 6791 | C | ALA | 1006 | | | -13.639 | 11.963 | 1.00 14.06 |
| ATOM | 6792 | Ö | ALA | 1006 | | | -14.703 | 11.864 | 1.00 13.17 |
| ATOM | 6793 | N | GLY | 1007 | | | -13.399 | 11.280 | 1.00 11.67 |
| ATOM | 6794 | CA | GLY | 1007 | | | -14.384 | 10.336 | 1.00 13.30 |
| ATOM | 6795 | C | GLY | 1007 | | | -14.701 | 10.358 | 1.00 11.83 |
| ATOM | 6796 | 0 | GLY | 1007 | | | -15.400 | 9.474 | 1.00 13.69 |
| MOTA | 6797 | N | ALA | 1008 | | | -14.183 | 11.354 | 1.00 10.96 |
| MOTA | 6798 | CA | ALA | 1008 | | | -14.430 | 11.484 | 1.00 10.68 |
| MOTA | 6799 | CB | ALA | 1008 | | | -14.059 | 12.894 | 1.00 11.65 |
| MOTA | 6800 | С | ALA | 1008 | | | -13.665 | 10.453 | 1.00 13.14 |
| MOTA | 6801 | 0 | ALA | 1008 | | | -12.624 | 9.951 | 1.00 14.60 |
| ATOM | 6802 | N | ASN | 1009 | | | -14.192 | 10.151 | 1.00 12.15 |
| ATOM | 6803 | CA | ASN | 1009 | | | -13.567 | 9.200 | 1.00 11.79 |
| ATOM | 6804 | CB | ASN | 1009 | | -9.652 | -14.579 | 8.197 | 1.00 13.02 |

| ATOM | 6805 | CG | ASN | 1009 | -8.583 | -15.225 | 7.376 | 1.00 13.44 |
|--------|------|-----|----------------------|------|---------|---------|--------|------------|
| ATOM | 6806 | OD1 | | 1009 | | -14.559 | 6.664 | 1.00 15.40 |
| ATOM | 6807 | ND2 | | 1009 | | -16.550 | 7.457 | 1.00 10.54 |
| | | C | ASN | 1009 | -10.327 | | 9.954 | 1.00 10.34 |
| ATOM | 6808 | | | | | | 9.429 | 1.00 11.35 |
| ATOM | 6809 | 0 | ASN | 1009 | -11.119 | | | |
| MOTA | 6810 | N | MET | 1010 | -10.493 | | 11.177 | 1.00 11.61 |
| MOTA | 6811 | CA | MET | 1010 | -11.660 | | 11.956 | 1.00 12.67 |
| ATOM | 6812 | CB | MET | 1010 | -12.824 | -14.052 | 11.513 | 1.00 10.94 |
| ATOM | 6813 | CG | MET | 1010 | -14.101 | -13.892 | 12.297 | 1.00 16.45 |
| ATOM | 6814 | SD | MET | 1010 | -15.423 | -14.958 | 11.623 | 1.00 18.40 |
| ATOM | 6815 | CE | MET | 1010 | -16.334 | -13.742 | 10.618 | 1.00 17.91 |
| MOTA | 6816 | С | MET | 1010 | -11.357 | -13.364 | 13.431 | 1.00 12.79 |
| ATOM | 6817 | 0 | MET | 1010 | | -14.207 | 13.792 | 1.00 10.90 |
| ATOM | 6818 | N | VAL | 1011 | -12.005 | | 14.276 | 1.00 11.92 |
| ATOM | 6819 | CA | VAL | 1011 | -11.787 | | 15.701 | 1.00 12.96 |
| ATOM | 6820 | CB | VAL | 1011 | -11.327 | | 16.246 | 1.00 14.64 |
| ATOM | 6821 | | VAL | 1011 | | -11.331 | 17.739 | 1.00 21.61 |
| | | | | 1011 | | -10.951 | 15.668 | 1.00 14.08 |
| ATOM | 6822 | | VAL | | | | 16.397 | 1.00 11.60 |
| ATOM | 6823 | C | VAL | 1011 | | -13.121 | | |
| ATOM | 6824 | 0 | VAL | 1011 | -14.165 | | 15.978 | 1.00 11.44 |
| MOTA | 6825 | N | LYS | 1012 | -12.924 | | 17.436 | 1.00 11.24 |
| ATOM | 6826 | CA | LYS | 1012 | -14.088 | | 18.187 | 1.00 10.46 |
| MOTA | 6827 | CB | LYS | 1012 | | -15.928 | 18.292 | 1.00 12.52 |
| ATOM | 6828 | CG | LYS | 1012 | -15.317 | -16.422 | 19.124 | 1.00 14.74 |
| MOTA | 6829 | CD | LYS | 1012 | -15.735 | -17.857 | 18.795 | 1.00 15.78 |
| ATOM | 6830 | CE | LYS | 1012 | -14.687 | -18.869 | 19.223 | 1.00 14.61 |
| ATOM | 6831 | NZ | LYS | 1012 | -14.548 | -18.899 | 20.722 | 1.00 13.04 |
| ATOM | 6832 | С | LYS | 1012 | -14.050 | -13.810 | 19.590 | 1.00 11.96 |
| ATOM | 6833 | 0 | LYS | 1012 | -13.015 | | 20.261 | 1.00 13.92 |
| ATOM | 6834 | N | ILE | 1013 | -15.186 | | 20.028 | 1.00 12.31 |
| MOTA | 6835 | CA | ILE | 1013 | -15.292 | | 21.357 | 1.00 13.37 |
| MOTA | 6836 | СВ | ILE | 1013 | -15.325 | | 21.278 | 1.00 13.64 |
| ATOM | 6837 | CG2 | ILE | 1013 | -13.959 | | 20.802 | 1.00 13.46 |
| | | CG1 | | | -16.419 | | 20.313 | 1.00 13.40 |
| MOTA | 6838 | | ILE | 1013 | | | | , |
| ATOM | 6839 | CD1 | ILE | 1013 | -16.605 | -9.181 | 20.299 | 1.00 16.29 |
| MOTA | 6840 | C | ILE | 1013 | -16.540 | | 22.062 | 1.00 14.88 |
| MOTA | 6841 | 0 | ILE | 1013 | -17.538 | | 21.414 | 1.00 14.92 |
| MOTA | 6842 | N | GLU | 1014 | -16.475 | | 23.388 | 1.00 14.84 |
| MOTA | 6843 | CA | GLU | 1014 | -17.581 | | 24.199 | 1.00 17.49 |
| MOTA | 6844 | CB | GLU | 1014 | -17.039 | | 25.334 | 1.00 14.94 |
| MOTA | 6845 | CG | GLU | 1014 | -16.318 | -15.943 | 24.884 | 1.00 18.47 |
| ATOM | 6846 | CD | GLU | 1014 | -15.753 | -16.757 | 26.052 | 1.00 18.83 |
| ATOM | 6847 | OE1 | GLU | 1014 | -16.166 | -16.532 | 27.205 | 1.00 20.52 |
| MOTA | 6848 | OE2 | GLU | 1014 | -14.900 | -17.629 | 25.811 | 1.00 20.24 |
| MOTA | 6849 | С | GLU | 1014 | -18.441 | -12.722 | 24.818 | 1.00 17.91 |
| ATOM | 6850 | 0 | GLU | 1014 | -17.928 | -11.775 | 25.410 | 1.00 18.79 |
| ATOM | 6851 | N | GLY | 1015 | -19.755 | -12.862 | 24.704 | 1.00 19.87 |
| MOTA | 6852 | CA | GLY | 1015 | -20.623 | | 25.292 | 1.00 20.15 |
| ATOM | 6853 | C | GLY | 1015 | -21.824 | | 24.445 | 1.00 22.90 |
| MOTA | 6854 | Õ | GLY | 1015 | -21.869 | | 23.254 | 1.00 22.51 |
| ATOM | 6855 | N | GLY | 1016 | -22.802 | | 25.064 | 1.00 23.73 |
| | | CA | GLY | | -24.010 | | 24.345 | |
| MOTA | 6856 | | | | -24.190 | | 24.052 | 1.00 24.20 |
| ATOM | 6857 | C. | GLY | 1016 | | -9.048 | | 1.00 24.34 |
| ATOM | 6858 | 0 | GLY | 1016 | -23.329 | -8.408 | 23:448 | |
| ATOM | 6859 | N | GLU | 1017 | -25.329 | -8.518 | 24.486 | 1.00 24.54 |
| ATOM | 6860 | CA | GLU | 1017 | -25.685 | -7.118 | 24.273 | 1.00 25.84 |
| ATOM | 6861 | CB | GLU | 1017 | -26.866 | -6.730 | 25.170 | 1.00 29.29 |
| ATOM | 6862 | CG | GLU · | 1017 | -28.235 | | 24.538 | 1.00 37.68 |
| ATOM | 6863 | CD | GLU | 1017 | -28.601 | -5.692 | 23.644 | 1.00 39.61 |
| MOTA | 6864 | OE1 | | 1017 | -27.961 | -5.504 | 22.590 | 1.00 39.67 |
| MOTA | 6865 | OE2 | GLU | 1017 | -29.533 | -4.943 | 24.012 | 1.00 43.46 |
| MOTA | 6866 | С | GLU | 1017 | -24.565 | -6.113 | 24.499 | 1.00 22.37 |
| MOTA | 6867 | 0 | GLU | 1017 | -24.354 | -5.229 | 23.673 | 1.00 20.28 |
| ATOM | 6868 | N | TRP | 1018 | -23.857 | -6.240 | 25.617 | 1.00 21.77 |
| ATOM ` | 6869 | CA | TRP | 1018 | -22.794 | -5.295 | 25.939 | 1.00 20.32 |
| ATOM | 6870 | CB | TRP | 1018 | -22.173 | -5.621 | 27.309 | 1.00 20.17 |
| ATOM | 6871 | CG | TRP | 1018 | -21.268 | -6.820 | 27.342 | 1.00 18.75 |
| ATOM | 6872 | CD2 | TRP | 1018 | -19.835 | -6.807 | 27.366 | 1.00 18.11 |
| ATOM | 6873 | CE2 | TRP | 1018 | -19.405 | -8.151 | 27.412 | 1.00 18.06 |
| ATOM | 6874 | CE3 | TRP | 1018 | -18.872 | -5.790 | 27.350 | 1.00 16.22 |
| ATOM | 6875 | | TRP | 1018 | -21.640 | -8.129 | 27.330 | 1.00 10.22 |
| | | | | | -20.527 | -8.938 | 27.373 | 1.00 20.28 |
| ATOM | 6876 | NE1 | TRP | 1018 | -18.049 | | 27.420 | 1.00 20.28 |
| ATOM | 6877 | CZ2 | TRP | 1018 | | -8.506 | | |
| ATOM | 6878 | CZ3 | TRP | 1018 | -17.523 | -6.146 | 27.384 | 1.00 17.33 |
| ATOM | 6879 | CH2 | TRP | 1018 | -17.129 | -7.495 | 27.430 | 1.00 16.12 |
| ATOM | 6880 | С | TRP | 1018 | -21.692 | -5.171 | 24.896 | 1.00 18.60 |
| ATOM | 6881 | 0 | TRP | 1018 | -20.943 | -4.193 | 24.901 | 1.00 20.29 |

| ATOM | 6882 | N | LEU | 1019 | -21.612 | -6.143 | 23.992 | 1.00 17.89 |
|-------|------|------|-------|------|---------|--------|--------|------------|
| ATOM | 6883 | CA | LEU | 1019 | -20.591 | -6.150 | 22.942 | 1.00 18.29 |
| ATOM | 6884 | CB | LEU | 1019 | -20.134 | -7.581 | 22.671 | 1.00 18.15 |
| ATOM | 6885 | CG | LEU | 1019 | -19.257 | -8.224 | 23.742 | 1.00 18.92 |
| ATOM | 6886 | CD1 | | 1019 | -18.970 | -9.657 | 23.341 | 1.00 18.85 |
| ATOM | 6887 | CD2 | LEU | 1019 | -17.969 | -7.431 | 23.886 | 1.00 17.98 |
| ATOM | 6888 | C | LEU | 1019 | -21.024 | -5.538 | 21.613 | 1.00 19.71 |
| | 6889 | 0 | LEU | 1019 | -20.206 | -5.395 | 20.707 | 1.00 13.71 |
| ATOM | | | | | -22.301 | -5.190 | 21.496 | 1.00 19.00 |
| ATOM | 6890 | N | VAL | 1020 | | | | |
| ATOM | 6891 | CA | VAL | 1020 | -22.833 | -4.612 | 20.272 | 1.00 19.17 |
| ATOM | 6892 | CB | VAL | 1020 | -24.281 | -4105 | 20.489 | 1.00 20.01 |
| ATOM | 6893 | | VAL | 1020 | -24.714 | -3.204 | 19.347 | 1.00 18.49 |
| ATOM | 6894 | CG2 | VAL | 1020 | -25.224 | -5.301 | 20.579 | 1.00 19.83 |
| MOTA | 6895 | C | VAL | 1020 | -21.987 | -3.478 | 19.708 | 1.00 20.01 |
| MOTA | 6896 | 0 | VAL | 1020 | -21.596 | -3.505 | 18.540 | 1.00 20.16 |
| MOTA | 6897 | N | GLU | 1021 | -21.697 | -2.486 | 20.539 | 1.00 20.60 |
| ATOM | 6898 | CA | GLU | 1021 | -20.899 | -1.351 | 20.107 | 1.00 21.01 |
| ATOM | 6899 | CB | GLU | 1021 | -20.744 | -0.355 | 21.254 | 1.00 26.20 |
| ATOM | 6900 | CG | GLU | 1021 | -19.763 | 0.761 | 20.952 | 1.00 30.81 |
| ATOM | 6901 | CD | GLU | 1021 | -19.791 | 1.857 | 21.994 | 1.00 35.68 |
| MOTA | 6902 | OE1 | GLU | 1021 | -19.602 | 1.551 | 23.193 | 1.00 38.35 |
| ATOM | 6903 | OE2 | GLU | 1021 | -20.002 | 3.026 | 21.606 | 1.00 38.75 |
| ATOM | 6904 | С | GLU | 1021 | -19.523 | -1.772 | 19.606 | 1.00 19.64 |
| ATOM | 6905 | 0 | GLU | 1021 | -19.062 | -1.327 | 18.555 | 1.00 18.56 |
| ATOM | 6906 | N | THR | 1022 | -18.862 | -2.624 | 20.375 | 1.00 18.69 |
| ATOM | 6907 | CA | THR | 1022 | -17.539 | -3.107 | 20.010 | 1.00 17.98 |
| ATOM | 6908 | СВ | THR | 1022 | -17.001 | -4.052 | 21.103 | 1.00 18.81 |
| MOTA | 6909 | OG1 | THR | 1022 | -16.885 | | 22.329 | 1.00 16.49 |
| ATOM | 6910 | CG2 | THR | 1022 | -15.633 | -4.606 | 20.721 | 1.00 17.33 |
| ATOM | 6911 | C | THR | 1022 | -17.575 | -3.831 | 18.664 | 1.00 17.26 |
| ATOM | 6912 | ō | THR | 1022 | -16.707 | -3.630 | 17.808 | 1.00 17.20 |
| | 6913 | | | 1022 | -18.588 | -4.670 | 18.478 | 1.00 10.30 |
| MOTA | | N | VAL | | | | 17.232 | 1.00 17.37 |
| ATOM | 6914 | CA | VAL | 1023 | -18.742 | -5.415 | | |
| ATOM | 6915 | CB | VAL | 1023 | -19.918 | -6.402 | 17.317 | 1.00 16.32 |
| ATOM | 6916 | | VAL | 1023 | -20.170 | -7.033 | 15.937 | 1.00 19.55 |
| ATOM | 6917 | CG2 | VAL | 1023 | -19.606 | -7.484 | 18.338 | 1.00 17.66 |
| MOTA | 6918 | С | VAL | 1023 | -18.972 | -4.484 | 16.048 | 1.00 18.30 |
| ATOM | 6919 | 0 | VAL | 1023 | -18.386 | -4.666 | 14.976 | 1.00 16.65 |
| MOTA | 6920 | N | GLN | 1024 | -19.828 | -3.488 | 16.242 | 1.00 18.44 |
| MOTA | 6921 | CA | GLN | 1024 | -20.125 | -2.540 | 15.169 | 1.00 20.28 |
| ATOM | 6922 | CB | GLN | 1024 | -21.152 | -1.498 | 15.631 | 1.00 22.35 |
| ATOM | 6923 | CG | GLN | 1024 | -22,494 | -2.088 | 16.057 | 1.00 28.92 |
| MOTA | 6924 | CD | GLN | 1024 | -23.512 | -1.029 | 16.479 | 1.00 31.59 |
| MOTA | 6925 | OE1 | GLN | 1024 | -23.238 | -0.195 | 17.349 | 1.00 32.26 |
| ATOM | 6926 | NE2 | GLN | 1024 | -24.700 | -1.069 | 15.871 | 1.00 31.37 |
| MOTA | 6927 | С | GLN | 1024 | -18.841 | -1.840 | 14.740 | 1.00 18.28 |
| ATOM | 6928 | 0 | GLN | 1024 | -18.519 | -1.791 | 13.554 | 1.00 19.29 |
| ATOM | 6929 | N | MET | 1025 | -18.104 | -1.319 | 15.717 | 1.00 16.21 |
| MOTA | 6930 | CA | MET | 1025 | -16.866 | -0.608 | 15.445 | 1.00 16.11 |
| ATOM | 6931 | CB | MET | 1025 | -16.388 | 0.105 | 16.716 | 1.00 17.05 |
| MOTA | 6932 | CG | MET | 1025 | -17.392 | 1.124 | 17.243 | 1.00 19.13 |
| ATOM | 6933 | SD | MET | 1025 | -16.834 | 1.990 | 18.708 | 1.00 22.52 |
| ATOM | 6934 | CE | MET | 1025 | -15.842 | 3.246 | 17.969 | 1.00 20.06 |
| ATOM | 6935 | c | MET | 1025 | -15.761 | -1.493 | 14.871 | 1.00 15.89 |
| ATOM | 6936 | Ō | MET | 1025 | -15.026 | -1.070 | 13.978 | 1.00 15.39 |
| ATOM | 6937 | N | LEU | 1026 | -15.630 | -2.719 | 15.374 | 1.00 15.63 |
| ATOM | 6938 | CA | LEU | 1026 | -14.602 | -3.614 | 14.852 | 1.00 14.77 |
| MOTA | 6939 | CB | LEU | 1026 | | -4.970 | 15.563 | 1.00 13.09 |
| ATOM | 6940 | CG | LEU | 1026 | -13.841 | -4.992 | 16.852 | 1.00 12.23 |
| ATOM | 6941 | | LEU | 1026 | -14.160 | -6.247 | 17.654 | 1.00 10.28 |
| ATOM | 6942 | | LEU | 1026 | -12.354 | -4.920 | 16.493 | 1.00 9.62 |
| ATOM | 6943 | C | LEU | 1026 | -14.771 | -3.821 | 13.353 | 1.00 15.22 |
| | | | | | -13.810 | -3.709 | 12.588 | 1.00 13.79 |
| ATOM | 6944 | 0 | LEU | 1026 | -16.003 | -4.115 | 12.947 | 1.00 13.79 |
| ATOM. | 6945 | N | THR | 1027 | | | | 1.00 23.03 |
| ATOM | 6946 | CA | THR | 1027 | -16.337 | -4.344 | 11.544 | 1.00 25.20 |
| ATOM | 6947 | CB | THR | 1027 | -17.863 | -4.600 | 11.369 | |
| ATOM | 6948 | OG1 | | 1027 | -18.251 | -5.736 | 12.150 | 1.00 29.61 |
| MOTA | | .CG2 | THR . | 1027 | -18.198 | -4.884 | 9.905 | 1.00 30.36 |
| MOTA | 6950 | C | THR | 1027 | -15.923 | -3.177 | 10.645 | 1.00 23.34 |
| MOTA | 6951 | 0 | THR | 1027 | -15.251 | -3.378 | 9.630 | 1.00 21.92 |
| MOTA | 6952 | N | GLU | 1028 | -16.315 | -1.957 | 11.005 | 1.00 23.53 |
| MOTA | 6953 | CA | GLU | 1028 | -15.945 | -0.807 | 10.181 | 1.00 24.72 |
| MOTA | 6954 | CB | GLU | 1028 | -16.678 | 0.466 | 10.643 | 1.00 27.14 |
| MOTA | 6955 | CG | GLU | 1028 | -17.060 | 0.487 | 12.105 | 1.00 28.12 |
| MOTA | 6956 | CD | GLU | 1028 | -17.832 | 1.740 | 12.511 | 1.00 25.37 |
| MOTA | 6957 | OE1 | GLU | 1028 | -18.914 | 2.007 | 11.949 | 1.00 26.88 |
| MOTA | 6958 | OE2 | GLU | 1028 | -17.362 | 2.462 | 13.408 | 1.00 24.11 |

| MOTA | 6959 | С | GLU | 1028 | -14.433 | -0.597 | 10.173 | 1.00 24.26 |
|--------------|-------------------|-----------|------------|--------------|--------------------|--------------------|------------------|--------------------------|
| ATOM | 6960 | 0 | GLU | 1028 | -13.895 | 0.084 | 9.299 | 1.00 24.65 |
| ATOM | 6961 | N | ARG | 1029 | -13.740 | -1.196 | 11.137 | 1.00 21.79 |
| MOTA | 6962 | CA | ARG | 1029 | -12.295 | -1.075 | 11.178 | 1.00 19.58 |
| ATOM | 6963 | CB | ARG | 1029 | -11.830 | -0.831 | 12.613 | 1.00 18.96 |
| ATOM | 6964 | CG | ARG | 1029 | -12.242 | 0.557 | 13.083 | 1.00 20.16 |
| MOTA | 6965 | CD | ARG | 1029 | -12.178 -12.643 | 0.735 2.075 | 14.577 14.944 | 1.00 16.37 1.00 18.38 |
| MOTA ATOM | 6966 6967 | NE CZ | ARG ARG | 1029 1029 | -12.843 | 2.524 | 14.749 | 1.00 15.38 |
| ATOM | 6968 | | ARG | 1029 | -14.800 | 1.745 | 14.192 | 1.00 15.81 |
| ATOM | 6969 | | ARG | 1029 | -14.202 | 3.762 | 15.104 | 1.00 17.73 |
| ATOM | 6970 | С | ARG | 1029 | -11.613 | -2.290 | 10.548 | 1.00 18.96 |
| MOTA | 6971 | 0 | ARG | 1029 | -10.479 | -2.628 | 10.882 | 1.00 18.45 |
| MOTA | 6972 | N | ALA | 1030 | -12.341 | -2.939 | 9.638 | 1.00 18.34 |
| ATOM | 6973 | CA | ALA | 1030 | -11.849 | -4.081 | 8.869 | 1.00 16.44 |
| MOTA | 6974 | СВ | ALA | 1030 | -10.532 | -3.702 | 8.187 | 1.00 17.45 |
| ATOM | 6975 | C | ALA | 1030 | -11.683 | -5.404 | 9.599 | 1.00 15.43 |
| MOTA | 6976 | 0 | ALA | 1030 | -11.004 | -6.292 | 9.094 | 1.00 15.15 |
| ATOM ATOM | 6977 6978 | N CA | VAL VAL | 1031 1031 | -12.305 -12.205 | -5.544 -6.783 | 10.766 11.529 | 1.00 14.41 1.00 14.99 |
| ATOM | 6979 | CB | VAL | 1031 | -11.741 | -6.513 | 12.990 | 1.00 14.99 |
| ATOM | 6980 | | VAL | 1031 | -11.731 | -7.811 | 13.792 | 1.00 15.39 |
| ATOM | 6981 | CG2 | VAL | 1031 | -10.351 | -5.899 | 12.988 | 1.00 16.52 |
| ATOM | 6982 | С | VAL | 1031 | -13.523 | -7.548 | 11.587 | 1.00 14.09 |
| ATOM | 6983 | 0 | VAL | 1031 | -14.499 | -7.074 | 12.175 | 1.00 14.29 |
| ATOM | 6984 | N | PRO | 1032 | -13.581 | -8.726 | 10.941 | 1.00 13.45 |
| ATOM | 6985 | CD | PRO | 1032 | -12.645 | -9.221 | 9.920 | 1.00 14.69 |
| MOTA | 6986 | CA | PRO | 1032 | -14.806 | -9.532 | 10.965 | 1.00 13.56 |
| MOTA | 6987 | CB | PRO | 1032 | -14.605 | | 9.827 | 1.00 13.39 |
| ATOM | 6988 | CG | PRO | 1032 | -13.133 | -10.622 | 9.698 | 1.00 19.95 |
| ATOM | 6989 | C | PRO | 1032 | -14.872 -13.850 | -10.187 | 12.337 12.905 | 1.00 13.75 1.00 14.39 |
| ATOM ATOM | 6990. 6991 | O N | PRO VAL | 1032 1033 | -13.850 | -10.572 -10.298 | 12.905 | 1.00 14.39 |
| ATOM | 6992 | CA | VAL | 1033 | | -10.236 | 14.200 | 1.00 13.00 |
| MOTA | 6993 | CB | VAL | 1033 | -16.871 | -9.776 | 15.137 | 1.00 13.98 |
| MOTA | 6994 | CG1 | | 1033 | -17.112 | -10.343 | 16.534 | 1.00 12.93 |
| MOTA | 6995 | CG2 | VAL | 1033 | -15.968 | -8.566 | 15.189 | 1.00 12.31 |
| MOTA | 6996 | С | VAL | 1033 | -17.175 | -12.047 | 14.239 | 1.00 14.20 |
| MOTA | 6997 [.] | 0 | VAL | 1033 | -18.219 | -12.078 | 13.580 | 1.00 13.95 |
| MOTA | 6998 | N | CYS | 1034 | -16.768 | | 15.019 | 1.00 12.45 |
| MOTA | 6999 | CA | CYS | 1034 | -17.577 | | 15.222 | 1.00 14.01 |
| ATOM | 7000 | CB | CYS | 1034 | -16.739 | -15.504 | 15.078 | 1.00 12.96 |
| MOTA MOTA | 7001 7002 | SG C | CYS CYS | 1034 1034 | -17.660 -18.057 | -17.005 | 15.555 16.661 | 1.00 15.25 1.00 13.22 |
| MOTA | 7002 | 0 | CYS | 1034 | -17.251 | | 17.569 | 1.00 13.22 |
| MOTA | 7004 | N | GLY | 1035 | -19.370 | | 16.850 | 1.00 13.48 |
| MOTA | 7005 | CA | GLY | 1035 | -19.940 | | 18.172 | 1.00 15.44 |
| MOTA | 7006 | С | GLY | 1035 | -19.826 | -15.397 | 18.897 | 1.00 15.74 |
| MOTA | 7007 | 0 | GLY | 1035 | -19.491 | | 18.294 | 1.00 16.26 |
| MOTA | 7008 | N | HIS | 1036 | -20.107 | | 20.196 | 1.00 15.37 |
| ATOM | 7009 | CA | HIS | 1036 | -20.027 | | 21.030 | 1.00 15.58 |
| ATOM | 7010 | CB | HIS | 1036 | -18.582 | | 21.507 | 1.00 16.13 |
| MOTA | 7011 | CG | HIS | 1036 | -18.335 | | 22.246 | 1.00 17.83 1.00 19.01 |
| MOTA MOTA | 7012 7013 | | HIS HIS | 1036 1036 | -19.187 -17.065 | | 22.755 22.525 | 1.00 19.01 |
| ATOM | 7014 | | HIS | 1036 | -17.145 | | 23.171 | 1.00 20.16 |
| ATOM | 7015 | | HIS | 1036 | -18.422 | | 23.324 | 1.00 18.10 |
| MOTA | 7016 | С | HIS | 1036 | -20.971 | | 22.223 | 1.00 15.56 |
| ATOM | 7017 | 0 | HIS | 1036 | -20.705 | -15.616 | 23.135 | 1.00 14.91 |
| MOTA | 7018 | N | LEU | 1037 | -22.072 | | 22.201 | 1.00 14.85 |
| MOTA | 7019 | CA | LEU | 1037 | -23.079 | | 23.254 | 1.00 19.01 |
| ATOM | 7020 | CB | LEU | 1037 | -24.404 | | 22.685 | 1.00 19.62 |
| ATOM | 7021 | CG | LEU | 1037 | -24.384 | | 22.079 | 1.00 20.40 |
| MOTA | 7022 | | LEU | 1037 | -25.681 | | 21.323 23.196 | 1.00 21.01 1.00 22.34 |
| ATOM ATOM | 7023 7024 | CD2 | LEU | 1037 1037 | -24.184 -23.327 | | 23.196 | 1.00 22.34 |
| ATOM | 7024 | 0 | LEU | 1037 | -23.327 | | 23.320 | 1.00 20.02 |
| ATOM | 7026 | N | GLY | 1038 | -23.967 | | 25.048 | 1.00 22.55 |
| ATOM | 7027 | CA | GLY | 1038 | -24.271 | | 25.764 | 1.00 25.04 |
| MOTA | 7028 | С | GLY | 1038 | -23.304 | | 26.909 | 1.00 26.30 |
| MOTA | 7029 | 0 | GLY | 1038 | -23.171 | | 27.767 | 1.00 27.66 |
| MOTA | 7030 | N | LEU | 1039 | -22.619 | | 26.925 | 1.00 28.14 |
| MOTA | 7031 | CA | LEU | 1039 | -21.655 | , | 27.976 | 1.00 29.16 |
| ATOM | 7032 | CB | LEU | 1039 | -21.525 | | 28.173 | 1.00 31.16 |
| ATOM | 7033 | CG CD1 | LEU | 1039 | -20.968 | | 29.503 29.570 | 1.00 33.32 1.00 35.58 |
| ATOM ATOM | 7034 7035 | | LEU LEU | 1039 1039 | -21.160 -19.503 | | 29.570 | 1.00 35.38 |
| | , 555 | CD2 | | _000 | 17.505 | | | |

| ATOM | 7036 | С | LEU | 1039 | -20.310 | -20.600 | 27.580 | 1.00 28.75 |
|------|------|------|-----|------|---------|---------|--------|------------|
| ATOM | 7037 | 0 | LEU | 1039 | -19.542 | -21.188 | 26.820 | 1.00 30.49 |
| | | | | | -20.049 | -19.397 | 28.085 | 1.00 29.32 |
| ATOM | 7038 | N | THR | 1040 | | | | |
| ATOM | 7039 | CA | THR | 1040 | -18.806 | -18.677 | 27.806 | 1.00 29.10 |
| ATOM | 7040 | CB | THR | 1040 | -19.043 | -17.147 | 27.758 | 1.00 30.20 |
| ATOM | 7041 | OG1 | THR | 1040 | -19.892 | -16.753 | 28.844 | 1.00 29.44 |
| ATOM | 7042 | CG2 | THR | 1040 | | -16.746 | 26.445 | 1.00 32.08 |
| | | | | | | | | |
| ATOM | 7043 | С | THR | 1040 | | -18.999 | 28.893 | 1.00 28.48 |
| ATOM | 7044 | 0 | THR | 1040 | -17.808 | -18.420 | 29.980 | 1.00 29.20 |
| MOTA | 7045 | N | PRO | 1041 | -16.850 | -19.920 | 28.597 | 1.00 28.41 |
| ATOM | 7046 | CD | PRO | 1041 | | -20.464 | 27.246 | 1.00 28.58 |
| | 7047 | | PRO | 1041 | -15.797 | | 29.518 | 1.00 27.50 |
| ATOM | | CA | | | | | | |
| ATOM | 7048 | CB | PRO | 1041 | | -21.298 | 28.652 | 1.00 28.87 |
| ATOM | 7049 | CG | PRO | 1041 | -15.152 | -20.773 | 27.279 | 1.00 32.35 |
| ATOM | 7050 | С | PRO | 1041 | -14.972 | -19.275 | 30.206 | 1.00 26.35 |
| ATOM | 7051 | 0 | PRO | 1041 | -14.484 | -19.479 | 31.320 | 1.00 24.47 |
| ATOM | 7052 | N | GLN | 1042 | -14.802 | -18.126 | 29.558 | 1.00 23.87 |
| | | | | | | | 30.188 | 1.00 23.26 |
| MOTA | 7053 | CA | GLN | 1042 | -14.043 | -17.050 | | |
| MOTA | 7054 | CB | GLN | 1042 | -13.872 | -15.868 | 29.223 | 1.00 22.94 |
| ATOM | 7055 | CG | GLN | 1042 | -12.682 | -16.011 | 28.273 | 1.00 19.12 |
| ATOM | 7056 | CD | GLN | 1042 | -12.640 | -14.915 | 27.228 | 1.00 22.27 |
| ATOM | 7057 | OE1 | GLN | 1042 | | -13.792 | 27.478 | 1.00 21.44 |
| | 7058 | NE2 | GLN | 1042 | | -15.231 | 26.049 | 1.00 19.01 |
| MOTA | | | | | | | | |
| ATOM | 7059 | C | GLN | 1042 | | -16.597 | 31.475 | 1.00 22.74 |
| ATOM | 7060 | 0 | GLN | 1042 | | -16.144 | 32.410 | 1.00 22.65 |
| ATOM | 7061 | N | SER | 1043 | -16.059 | -16.739 | 31.532 | 1.00 24.41 |
| ATOM | 7062 | CA | SER | 1043 | | -16.339 | 32.723 | 1.00 24.75 |
| ATOM | 7063 | CB | SER | 1043 | | -15.799 | 32.326 | 1.00 26.59 |
| | | | | | | | | |
| MOTA | 7064 | OG | SER | 1043 | -18.069 | -14.611 | 31.563 | 1.00 29.05 |
| MOTA | 7065 | С | SER | 1043 | -16.981 | -17.493 | 33.710 | 1.00 24.52 |
| ATOM | 7066 | 0 | SER | 1043 | -17.845 | -17.440 | 34.581 | 1.00 25.87 |
| ATOM | 7067 | N | VAL | 1044 | | -18.524 | 33.578 | 1.00 23.32 |
| ATOM | 7068 | CA | VAL | 1044 | -16.227 | -19.695 | 34.454 | 1.00 22.51 |
| | | | | | | | | |
| MOTA | 7069 | СВ | VAL | 1044 | -15.004 | -20.632 | 34.249 | 1.00 23.18 |
| MOTA | 7070 | CG1 | | 1044 | -13.718 | -19.911 | 34.614 | 1.00 22.95 |
| ATOM | 7071 | CG2 | VAL | 1044 | -15.166 | -21.895 | 35.084 | 1.00 22.94 |
| ATOM | 7072 | С | VAL | 1044 | -16.338 | -19.326 | 35.933 | 1.00 22.48 |
| ATOM | 7073 | 0 | VAL | 1044 | -17.060 | -19.982 | 36.682 | 1.00 23.24 |
| ATOM | 7074 | N | ASN | 1045 | -15.626 | -18.287 | 36.360 | 1.00 22.59 |
| ATOM | 7075 | CA | ASN | 1045 | | -17.879 | 37.761 | 1.00 24.64 |
| | | • | | | | -16.911 | 38.091 | 1.00 23.05 |
| ATOM | 7076 | CB | ASN | 1045 | -14.546 | | | |
| MOTA | 7077 | CG | ASN | 1045 | -13.187 | -17.545 | 37.913 | 1.00 21.46 |
| MOTA | 7078 | | ASN | 1045 | -12.806 | -18.447 | 38.666 | 1.00 20.69 |
| ATOM | 7079 | ND2 | ASN | 1045 | -12.453 | -17.096 | 36.904 | 1.00 20.14 |
| MOTA | 7080 | С | ASN | 1045 | -17.019 | -17.237 | 38.107 | 1.00 25.96 |
| MOTA | 7081 | 0 | ASN | 1045 | -17.458 | -17.289 | 39.257 | 1.00 26.58 |
| ATOM | 7082 | N | ILE | 1046 | -17.666 | -16.633 | 37.115 | 1.00 28.57 |
| ATOM | 7083 | CA | ILE | 1046 | -18.962 | -15.997 | 37.342 | 1.00 30.78 |
| ATOM | 7084 | CB | ILE | 1046 | -19.397 | -15.116 | 36.141 | 1.00 30.35 |
| | | | | | | | | |
| ATOM | 7085 | CG2 | ILE | 1046 | -20.822 | -14.616 | 36.356 | 1.00 29.76 |
| ATOM | 7086 | _CG1 | ILE | 1046 | -18.440 | -13.933 | 35.970 | 1.00 29.93 |
| MOTA | 7087 | CD1 | ILE | 1046 | -18.419 | -12.976 | 37.145 | 1.00 28.61 |
| ATOM | 7088 | С | ILE | 1046 | -20.023 | -17.067 | 37.551 | 1.00 32.86 |
| ATOM | 7089 | Ō | ILE | 1046 | -20.841 | -16.971 | 38.466 | 1.00 32.88 |
| | | | | | | -18.084 | | |
| ATOM | 7090 | N | PHE | 1047 | | | 36.693 | |
| ATOM | 7091 | CA | PHE | 1047 | | -19.174 | 36.783 | 1.00 39.34 |
| MOTA | 7092 | CB | PHE | 1047 | | -19.878 | 35.430 | 1.00 40.96 |
| MOTA | 7093 | CG | PHE | 1047 | -21.373 | -18.946 | 34.277 | 1.00 43.16 |
| ATOM | 7094 | CD1 | PHE | 1047 | | -18.029 | 34.313 | 1.00 45.03 |
| ATOM | 7095 | CD2 | PHE | 1047 | | -19.003 | 33.141 | 1.00 44.64 |
| | | | | | | | | |
| MOTA | 7096 | CE1 | PHE | 1047 | | -17.177 | 33.234 | 1.00 45.71 |
| MOTA | 7097 | CE2 | PHE | 1047 | | -18.157 | 32.057 | 1.00 45.87 |
| MOTA | 7098 | CZ | PHE | 1047 | -21.851 | -17.243 | 32.104 | 1.00 46.15 |
| ATOM | 7099 | С | PHE | 1047 | -20.559 | -20.204 | 37.829 | 1.00 40.40 |
| MOTA | 7100 | 0 | PHE | 1047 | | -20.982 | 38.309 | 1.00 40.84 |
| ATOM | 7101 | N | GLY | 1048 | -19.275 | -20.208 | 38.174 | 1.00 40.74 |
| ATOM | 7102 | CA | GLY | 1048 | -18.780 | -21.157 | 39.153 | 1.00 41.82 |
| | | | | | | | | |
| ATOM | 7103 | С | GLY | 1048 | | -22.550 | 38.561 | 1.00 43.00 |
| MOTA | 7104 | 0 | GLY | 1048 | | -23.546 | 39.220 | 1.00 42.75 |
| MOTA | 7105 | N | GLY | 1049 | -18.262 | -22.617 | 37.306 | 1.00 43.62 |
| ATOM | 7106 | CA | GLY | 1049 | -18.140 | -23.893 | 36.629 | 1.00 45.01 |
| MOTA | 7107 | C | GLY | 1049 | | -23.799 | 35.229 | 1.00 46.15 |
| ATOM | 7108 | ō | GLY | 1049 | | -22.723 | 34.800 | 1.00 45.08 |
| MOTA | | | | 1050 | -18.725 | | 34.513 | 1.00 47.77 |
| | 7109 | N | TYR | | | | | |
| MOTA | 7110 | CA | TYR | 1050 | | -24.940 | 33.156 | 1.00 49.51 |
| MOTA | 7111 | CB | TYR | 1050 | -18.312 | -25.707 | 32.227 | 1.00 49.59 |
| MOTA | 7112 | CG | TYR | 1050 | -16.897 | -25.181 | 32.246 | 1.00 49.48 |
| | | | | | | | | |

| ATOM | 7113 | CD1 | TYR | 1050 | -15.963 | -25.674 | 33.153 | 1.00 49.47 |
|------|-------|-----|-----|------|---------|---------|--------|-------------|
| ATOM | 7114 | CE1 | TYR | 1050 | -14.669 | -25.170 | 33.196 | 1.00 50.01 |
| ATOM | 7115 | CD2 | TYR | 1050 | -16.499 | -24.166 | 31.376 | 1.00 49.76 |
| ATOM | 7116 | CE2 | TYR | 1050 | -15.207 | -23.652 | 31.411 | 1.00 49.86 |
| ATOM | 7117 | CZ | TYR | 1050 | -14.298 | -24.159 | 32.323 | 1.00 50.33 |
| АТОМ | 7118 | ОН | TYR | 1050 | -13.019 | | 32.370 | 1.00 50.67 |
| ATOM | 7119 | C | TYR | 1050 | -20.635 | | 33.136 | 1.00 50.55 |
| ATOM | 7120 | ō | TYR | 1050 | -20.778 | | 32.876 | 1.00 50.84 |
| ATOM | 7121 | N | LYS | 1051 | -21.648 | | 33.412 | 1.00 51.54 |
| ATOM | 7122 | CA | LYS | 1051 | -23.031 | | 33.444 | 1.00 52.63 |
| ATOM | 7123 | CB | LYS | 1051 | -23.738 | | 34.662 | 1.00 53.67 |
| ATOM | 7123 | CG | LYS | 1051 | -22.963 | | 35.960 | 1.00 55.80 |
| | 7125 | CD | LYS | 1051 | -23.561 | | 37.087 | 1.00 56.82 |
| MOTA | 7126 | CE | | 1051 | -23.501 | | 38.328 | 1.00 57.73 |
| ATOM | | | LYS | | -23.192 | | 39.410 | 1.00 57.73 |
| MOTA | 7127 | NZ | LYS | 1051 | | -23.119 | 32.165 | 1.00 52.42 |
| ATOM | 7128 | C | LYS | 1051 | | | | |
| ATOM | 7129 | 0 | LYS | 1051 | -23.359 | | 31.495 | 1.00 51.97 |
| ATOM | 7130 | N | VAL | 1052 | -24.821 | | 31.832 | 1.00 52.32 |
| MOTA | 7131 | CA | VAL | 1052 | -25.595 | | 30.632 | 1.00 52.55 |
| ATOM | 7132 | CB | VAL | 1052 | -26.555 | | 30.299 | 1.00 51.86 |
| ATOM | 7133 | | VAL | 1052 | -27.330 | | 29.025 | 1.00 51.77 |
| ATOM | 7134 | | VAL | 1052 | -25.771 | | 30.147 | 1.00 51.56 |
| ATOM | 7135 | С | VAL | 1052 | -26.414 | | 30.779 | 1.00 52.86 |
| ATOM | 7136 | 0 | VAL | 1052 | -26.992 | | 31.834 | 1.00 52.72 |
| ATOM | 7137 | N | GLN | 1053 | -26.449 | | 29.714 | 1.00 53.38 |
| MOTA | 7138 | CA | GLN | 1053 | -27.207 | | 29.701 | 1.00 53.40 |
| ATOM | 7139 | CB | GLN | 1053 | -26.328 | | 29.234 | 1.00 53.64 |
| MOTA | 7140 | CG | GLN | 1053 | -25.598 | | 30.348 | 1.00 54.11 |
| ATOM | 7141 | CD | GLN | 1053 | -24.605 | | 31.081 | 1.00 53.82 |
| ATOM | 7142 | | GLN | 1053 | -23.756 | | | 1.00 55.31 |
| MOTA | 7143 | NE2 | GLN | 1053 | -24.697 | | 32.406 | 1.00 53.40 |
| ATOM | 7144 | С | GLN | 1053 | -28.410 | | 28.773 | 1.00 53.18 |
| MOTA | 7145 | 0 | GLN | 1053 | -28.560 | -23.043 | 28.070 | 1.00 52.32 |
| ATOM | 7146 | N | GLY | 1054 | -29.261 | -21.024 | 28.773 | 1.00 53.68 |
| MOTA | 7147 | CA | GLY | 1054 | -30.440 | -21.045 | 27.927 | 1.00 54.63 |
| MOTA | 7148 | С | GLY | 1054 | -31.592 | -21.795 | 28.567 | 1.00 55.39 |
| MOTA | 7149 | 0 | GLY | 1054 | -32.719 | -21.745 | 28.080 | 1.00 55.28 |
| ATOM | 7150 | N | ARG | 1055 | -31.303 | -22.495 | 29.660 | 1.00 56.01 |
| MOTA | 7151 | CA | ARG | 1055 | -32.314 | -23.255 | 30.382 | 1.00 57.40 |
| ATOM | 7152 | CB | ARG | 1055 | -31.674 | -24.003 | 31.556 | 1.00 59.12 |
| ATOM | 7153 | CG | ARG | 1055 | -30.714 | -25.123 | 31.166 | 1.00 61.02 |
| MOTA | 7154 | CD | ARG | 1055 | -31.455 | -26.328 | 30.604 | 1.00 62.44 |
| MOTA | 7155 | NE | ARG | 1055 | -30.566 | -27.459 | 30.347 | 1.00 63.71 |
| MOTA | 7156 | CZ | ARG | 1055 | -29.867 | -28.095 | 31.284 | 1.00 64.04 |
| ATOM | 7157 | NH1 | ARG | 1055 | -29.949 | -27.713 | 32.551 | 1.00 64.28 |
| ATOM | 7158 | NH2 | ARG | 1055 | -29.086 | -29.117 | 30.955 | 1.00 64.25 |
| ATOM | 7159 | С | ARG | 1055 | -33.403 | -22.325 | 30.911 | 1.00 57.48. |
| ATOM | 7160 | 0 | ARG | 1055 | -33.223 | -21.667 | 31.936 | 1.00 57.81 |
| ATOM | 7161 | N | GLY | 1056 | -34.530 | | 30.208 | 1.00 57.14 |
| MOTA | 7162 | CA | GLY | 1056 | -35.619 | | 30.643 | 1.00 56.84 |
| ATOM | 7163 | С | GLY | 1056 | -36.179 | | 29.552 | 1.00 56.31 |
| ATOM | 7164 | 0 | GLY | 1056 | -35.678 | | 28.427 | 1.00 55.89 |
| ATOM | 7165 | N | ASP | 1057 | | -19.778 | 29.894 | 1.00 56.37 |
| ATOM | 7166 | CA | ASP | 1057 | -37.869 | | 28.951 | 1.00 56.25 |
| ATOM | 7167 | СВ | ASP | 1057 | | -18.615 | 29.382 | 1.00 57.60 |
| ATOM | 7168 | CG | ASP | 1057 | | -19.886 | 29.450 | 1.00 58.32 |
| ATOM | 7169 | | ASP | 1057 | | -20.525 | 28.394 | 1.00 58.27 |
| ATOM | 7170 | OD2 | ASP | 1057 | -40.589 | | 30.560 | 1.00 58.42 |
| ATOM | 7171 | C | ASP | 1057 | -37.116 | | 28.868 | 1.00 55.73 |
| ATOM | 7172 | ō | ASP | 1057 | | -17.154 | 27.797 | 1.00 55.55 |
| MOTA | 7173 | N | GLU | 1058 | | -16.878 | 30.005 | 1.00 54.61 |
| ATOM | 7174 | CA | GLU | 1058 | | -15.600 | 30.059 | 1.00 53.66 |
| MOTA | 7175 | CB | GLU | 1058 | -36.187 | | 31.510 | 1.00 54.74 |
| MOTA | 7176 | CG | GLU | 1058 | -35.451 | | 31.680 | 1.00 56.54 |
| ATOM | 7177 | CD | GLU | 1058 | | -13.289 | 33.103 | 1.00 57.81 |
| ATOM | 7178 | OE1 | GLU | 1058 | -36.616 | | 33.560 | 1.00 58.07 |
| ATOM | 7179 | OE2 | GLU | 1058 | | -13.247 | 33.767 | 1.00 58.77 |
| MOTA | 7180 | C | GLU | 1058 | | -15.700 | 29.436 | 1.00 52.45 |
| ATOM | 7181 | ō | GLU | 1058 | | -14.950 | 28.515 | 1.00 52.76 |
| ATOM | 7182 | N | ALA | 1059 | | -16.628 | 29.937 | 1.00 50.76 |
| ATOM | 7183 | CA | ALA | 1059 | | -16.820 | 29.420 | 1.00 48.43 |
| ATOM | 7184 | CB | ALA | 1059 | | -17.834 | 30.277 | 1.00 48.71 |
| ATOM | 7185 | С | ALA | 1059 | | -17.290 | 27.969 | 1.00 46.48 |
| ATOM | 7186 | 0 | ALA | 1059 | | -16.913 | 27.153 | 1.00 46.02 |
| ATOM | 7187 | N | GLY | 1060 | | -18.116 | 27.658 | 1.00 44.48 |
| ATOM | 7188 | CA | GLY | 1060 | -33.763 | | 26.307 | 1.00 42.19 |
| ATOM | 7189 | CA | | 1060 | -34.145 | | 25.315 | 1.00 41.58 |
| | , 103 | C | GLY | 1000 | J4.14J | T 437 | | |

| ATOM | 7190 | 0 | GLY | 1060 | -33.539 | -17.480 | 24.245 | 1.00 41.81 |
|--------|--------|---------|------------|------|---------|---------|--------|--------------------------|
| ATOM | 7191 | N | ASP | 1061 | -35.008 | -16.540 | 25.667 | 1.00 40.06 |
| ATOM | 7192 | CA | ASP | 1061 | -35.288 | -15.401 | 24.797 | 1.00 38.77 |
| ATOM | 7193 | CB | ASP | 1061 | -36.570 | -14.686 | 25.236 | 1.00 39.86 |
| ATOM | 7194 | CG | ASP | 1061 | -37.760 | -15.616 | 25.318 | 1.00 39.94 |
| ATOM | 7195 | OD1 | ASP | 1061 | -38.037 | -16.323 | 24.328 | 1.00 40.73 |
| ATOM | 7196 | | ASP | 1061 | -38.422 | -15.634 | 26.375 | 1.00 41.22 |
| ATOM | 7197 | С | ASP | 1061 | -34.131 | | 24.837 | 1.00 37.48 |
| MOTA | 7198 | ō | ASP | 1061 | -33.857 | | 23.854 | 1.00 37.88 |
| ATOM | 7199 | N | GLN | 1062 | -33.464 | | 25.983 | 1.00 35.98 |
| ATOM | 7200 | CA | GLN | 1062 | -32.337 | | 26.155 | 1.00 34.74 |
| ATOM | 7201 | CB | GLN | 1062 | -31.807 | -13.508 | 27.586 | 1.00 35.48 |
| ATOM | 7202 | CG | GLN | 1062 | -30.679 | -12.533 | 27.895 | 1.00 36.93 |
| | 7202 | CD | GLN | 1062 | -31.115 | | 27.786 | 1.00 38.62 |
| ATOM | 7203 | OE1 | GLN | 1062 | -32.048 | | 28.465 | 1.00 38.65 |
| MOTA | 7204 | NE2 | | 1062 | -30.439 | | 26.933 | 1.00 38.92 |
| ATOM | | C | GLN | 1062 | -31.225 | | 25.173 | 1.00 33.19 |
| MOTA | 7206 | | GLN | | -30.671 | | 24.512 | 1.00 33.19 |
| ATOM | 7207 | 0 | GLN | 1062 | | | 25.082 | 1.00 31.37 |
| MOTA | 7208 | N | LEU | 1063 | -30.904 | | 24.176 | 1.00 32.49 |
| ATOM | 7209 | CA | LEU | 1063 | -29.861 | | 24.176 | |
| ATOM | 7210 | CB | LEU | 1063 | -29.584 | | | 1.00 32.31 1.00 33.38 |
| ATOM | 7211 | CG | LEU | 1063 | | -17.413 | 25.721 | |
| ATOM | 7212 | | LEU | 1063 | -28.693 | -18.923 | 25.776 | 1.00 34.58 |
| MOTA | 7213 | CD2 | LEU | 1063 | | -16.701 | 25.837 | 1.00 33.59 |
| ATOM | 7214 | C | LEU | 1063 | -30.243 | | 22.718 | 1.00 31.49 |
| MOTA | 7215 | 0 | LEU | 1063 | -29.410 | | 21.910 | 1.00 29.46 |
| MOTA | 7216 | N | LEU | 1064 | | -15.544 | 22.385 | 1.00 30.95 |
| MOTA | 7217 | CA | LEU | 1064 | -31.984 | | 21.024 | 1.00 31.20 |
| ATOM | 7218 | CB | LEU | 1064 | -33.442 | | 20.899 | 1.00 33.16 |
| ATOM | 7219 | CG | LEU | 1064 | -34.097 | | 19.513 | 1.00 34.91 |
| MOTA | 7220 | CD1 | LEU | 1064 | -35.286 | | 19.482 | 1.00 35.64 |
| MOTA | 7221 | CD2 | LEU | 1064 | -34.536 | | 19.182 | 1.00 34.56 |
| ATOM | 7222 | C | LEU | 1064 | -31.865 | | 20.696 | 1.00 29.59 |
| MOTA | 7223 | 0 | LEU | 1064 | -31.476 | | 19.589 | 1.00 28.93 |
| MOTA | 7224 | N | SER | 1065 | -32.191 | -13.009 | 21.672 | 1.00 27.94 |
| ATOM | 7225 | CA | SER | 1065 | -32.106 | -11.572 | 21.475 | 1.00 27.91 |
| ATOM | 7226 | CB | SER | 1065 | -32.645 | -10.830 | 22.697 | 1.00 28.13 |
| MOTA | 7227 | OG | SER | 1065 | -32.610 | -9.429 | 22.483 | 1.00 30.15 |
| ATOM | 7228 | C | SER | 1065 | -30.662 | -11.156 | 21.219 | 1.00 26.39 |
| ATOM | 7229 | 0 | SER | 1065 | -30.389 | -10.386 | 20.300 | 1.00 26.00 |
| ATOM · | 7230 | N | ASP | 1066 | -29.741 | -11.665 | 22.035 | 1.00 25.06 |
| ATOM | 7231 | CA | ASP | 1066 | -28.320 | -11.340 | 21.880 | 1.00 24.78 |
| ATOM | 7232 | CB | ASP | 1066 | -27.491 | -11.989 | 22.989 | 1.00 25.95 |
| ATOM | 7233 | CG | ASP | 1066 | -27.730 | -11.348 | 24.338 | 1.00 28.70 |
| ATOM | 7234 | OD1 | ASP | 1066 | -27.860 | -10.107 | 24.385 | 1.00 30.67 |
| MOTA | 7235 | OD2 | ASP | 1066 | -27.775 | -12.077 | 25.351 | 1.00 31.26 |
| ATOM | 7236 | С | ASP | 1066 | -27.783 | -11.782 | 20.524 | 1.00 23.52 |
| MOTA | 7237 | 0 | ASP | 1066 | -26.968 | -11.089 | 19.915 | 1.00 23.49 |
| ATOM | 7238 | N | ALA | 1067 | -28.235 | -12.945 | 20.062 | 1.00 23.51 |
| ATOM | 7239 | CA | ALA | 1067 | -27.813 | -13.478 | 18.776 | 1.00 22.29 |
| ATOM | 7240 | СВ | ALA | 1067 | -28.450 | -14.842 | 18.547 | 1.00 22.43 |
| ATOM | 7241 | С | ALA | 1067 | -28.216 | | 17.665 | 1.00 22.46 |
| ATOM | 7242 | 0 | ALA | 1067 | | -12.164 | 16.804 | 1.00 20.38 |
| ATOM | 7243 | N | LEU | 1068 | | -12.091 | 17.683 | 1.00 23.01 |
| MOTA | 7244 . | CA | LEU | 1068 | -29.961 | -11.167 | 16.668 | 1.00 22.75 |
| MOTA | 7245 | CB | LEU | 1068 | -31.464 | -10.947 | 16.844 | 1.00 22.25 |
| MOTA | 7246 | CG | LEU | 1068 | -32.364 | -12.126 | 16.480 | 1.00 23.59 |
| ATOM | 7247 | | LEU | 1068 | -33.765 | -11.876 | 17.028 | 1.00 25.32 |
| ATOM | 7248 | | LEU | 1068 | -32.399 | -12.310 | 14.959 | 1.00 24.63 |
| ATOM | 7249 | C | LEU | 1068 | -29.224 | -9.838 | 16.784 | 1.00 20.46 |
| ATOM | 7250 | ō | LEU | 1068 | -28.926 | -9.210 | 15.781 | 1.00 20.46 |
| ATOM | 7251 | N | ALA | 1069 | -28.928 | -9.436 | 18.016 | 1.00 20.31 |
| MOTA | 7252 | CA | ALA | 1069 | -28.234 | -8.186 | 18.284 | 1.00 20.51 |
| ATOM | 7253 | СВ | ALA | 1069 | -28.237 | -7.899 | 19.783 | 1.00 21.24 |
| ATOM | 7254 | C | ALA | 1069 | -26.803 | -8.201 | 17.757 | 1.00 18.78 |
| ATOM | 7255 | Ö | ALA | 1069 | -26.326 | -7.211 | 17.203 | 1.00 17.76 |
| ATOM | 7256 | N | LEU | 1070 | -26.117 | -9.325 | 17.929 | 1.00 19.42 |
| ATOM | 7257 | CA | LEU | 1070 | -24.745 | -9.440 | 17.455 | 1.00 18.83 |
| ATOM | 7258 | CB | LEU | 1070 | -24.743 | -10.719 | 18.005 | 1.00 18.63 |
| ATOM | 7259 | CG | LEU | 1070 | -23.813 | -10.713 | 19.516 | 1.00 17.66 |
| ATOM | 7260 | CD1 | LEU | 1070 | -23.361 | -12.111 | 19.965 | 1.00 17.08 |
| ATOM | 7261 | CD2 | LEU | 1070 | -22.750 | -9.689 | 19.849 | 1.00 17.00 |
| ATOM | 7262 | CD2 | LEU | 1070 | -24.741 | -9.435 | 15.930 | 1.00 10.40 |
| ATOM | 7262 | 0 | LEU | 1070 | -23.897 | -8.791 | 15.308 | 1.00 16.25 |
| ATOM | 7264 | | | 1070 | -25.692 | -10.141 | 15.327 | 1.00 10.23 |
| ATOM | 7265 | N CA | GLU GLU | 1071 | -25.789 | | 13.872 | 1.00 19.82 |
| ATOM | 7266 | CB | GLU | 1071 | -26.907 | | 13.445 | 1.00 22.79 |
| .11011 | ,200 | CD | 3110 | 10/1 | 20.507 | , | | |
| | | | | | | | | |

| ATOM | 7267 | CG GLU | 1071 | - | 27.158 | -11.196 | 11.944 | 1.00 23.57 |
|--------------|--------------|--------------------|--------------|---|--------|--------------------|------------------|--------------------------|
| ATOM | 7268 | CD GLU | 1071 | - | 28.293 | -12.133 | 11.587 | 1.00 25.87 |
| ATOM | 7269 | OE1 GLU | 1071 | - | 29.412 | -11.938 | 12.111 | 1.00 26.11 |
| ATOM | 7270 | OE2 GLU | 1071 | - | 28.075 | -13.063 | 10.783 | 1.00 27.62 |
| ATOM · | 7271 | C GLU | 1071 | - | 26.069 | -8.775 | 13.324 | 1.00 19.77 |
| ATOM | 7272 | O GLU | 1071 | - | 25.424 | -8.339 | 12.374 | 1.00 17.58 |
| ATOM | 7273 | N ALA | 1072 | - | 27.028 | -8.071 | 13.922 | 1.00 20.66 |
| ATOM | 7274 | CA ALA | 1072 | - | 27.368 | -6.721 | 13.467 | 1.00 20.74 |
| ATOM | 7275 | CB ALA | 1072 | - | 28.569 | -6.182 | 14.245 | 1.00 21.28 |
| ATOM | 7276 | C ALA | 1072 | - | 26.176 | -5.786 | 13.630 | 1.00 22.41 |
| ATOM | 7277 | O ALA | 1072 | - | 26.034 | -4.804 | 12.898 | 1.00 23.66 |
| MOTA | 7278 | N ALA | 1073 | - | 25.319 | -6.099 | 14.598 | 1.00 22.57 |
| MOTA | 7279 | CA ALA | 1073 | - | 24.130 | -5.295 | 14.856 | 1.00 19.20 |
| MOTA | 7280 | CB ALA | 1073 | - | 23.572 | -5.616 | 16.241 | 1.00 20.25 |
| MOTA | 7281 | C ALA | 1073 | - | 23.058 | -5.530 | 13.792 | 1.00 19.63 |
| MOTA | 7282 | O ALA | 1073 | - | 22.136 | -4.730 | 13.647 | 1.00 19.20 |
| MOTA | 7283 | N GLY | 1074 | - | 23.168 | -6.628 | 13.049 | 1.00 17.74 |
| ATOM | 7284 | CA GLY | 1074 | - | 22.175 | -6.890 | 12.018 | 1.00 17.83 |
| ATOM | 7285 | C GLY | 1074 | - | 21.454 | -8.225 | 12.112 | 1.00 17.24 |
| ATOM . | 7286 | O GLY | 1074 | | 20.632 | -8.545 | 11.250 | 1.00 17.98 |
| ATOM | 7287 | N ALA | 1075 | | 21.739 | -9.005 | 13.149 | 1.00 17.76 |
| MOTA | 7288 | CA ALA | 1075 | | | -10.310 | 13.286 | 1.00 17.79 |
| MOTA | 7289 | CB ALA | 1075 | | | -10.994 | 14.581 | 1.00 16.20 |
| MOTA | 7290 | C ALA | 1075 | | | -11.160 | 12.080 | 1.00 18.93 |
| ATOM | 7291 | O ALA | 1075 | | | -11.237 | 11.709 | 1.00 18.99 |
| ATOM | 7292 | n gln | 1076 | | | -11.790 | 11.468 | 1.00 17.65 |
| ATOM | 7293 | CA GLN | 1076 | | | -12.625 | 10.283 | 1.00 19.07 |
| MOTA | 7294 | CB GLN | 1076 | | | -12.363 | 9.258 | 1.00 20.10 |
| MOTA | 7295 | CG GLN | 1076 | | | -10.967 | 8.666 | 1.00 21.35 |
| ATOM | 7296 | CD GLN | 1076 | | | -10.664 | 7.700 | 1.00 23.80 |
| ATOM | 7297 | OE1 GLN | 1076 | | | -11.110 | 6.547 | 1.00 28.97 |
| ATOM | 7298 | NE2 GLN | 1076 | | 17.540 | -9.900 | 8.164 | 1.00 19.71 |
| MOTA | 7299 | C GLN | 1076 | | | -14.110 | 10.604 | 1.00 18.87 |
| MOTA | 7300 | O GLN | 1076 | | | -14.933 | 9.731 | 1.00 21.05 |
| MOTA | 7301 | N LEU | 1077 | | | -14.435 | 11.867 | 1.00 19.04 |
| ATOM | 7302 | CA LEU | 1077 | | | -15.804 | 12.361 | 1.00 18.01 |
| ATOM | 7303 | CB LEU | 1077 | | | -16.467 | 12.210 | 1.00 21.10 |
| MOTA | 7304 | CG LEU | 1077 | | | -17.310 | 10.966 | 1.00 22.57 |
| MOTA | 7305 | CD1 LEU | 1077 | | | -17.821 | 10.996 | 1.00 24.38 |
| ATOM | 7306 | CD2 LEU | 1077 | | | -18.477 | 10.920 | 1.00 23.84 |
| ATOM | 7307 | C LEU | 1077 | | | -15.799 | 13.831 | 1.00 17.60 |
| MOTA | 7308 | O LEU | 1077 | | | -14.816 | 14.536 | 1.00 17.24 |
| MOTA | 7309 | N LEU | 1078 | | | -16.895 | 14.293 | 1.00 16.91 |
| ATOM | 7310 | CA LEU | 1078 | | | -17.013 | 15.700 | 1.00 17.04 |
| ATOM | 7311 | CB LEU | 1078 | | | -16.631 | 15.904 | 1.00 18.53 |
| MOTA | 7312 | CG LEU | 1078 | | | -16.847 | 17.336 | 1.00 19.84 |
| MOTA | 7313 | CD1 LEU | 1078 | | | -15.825 | 18.288 | 1.00 19.36 |
| ATOM | 7314 | CD2 LEU | 1078 | | | -16.719 | 17.362 | 1.00 20.91 |
| ATOM | 7315 | C LEU | 1078 | | | -18.434 | 16.206 | 1.00 17.33 |
| ATOM | 7316 | O LEU | 1078 | | | -19.395 | 15.563 | 1.00 18.22 |
| ATOM | 7317 | N VAL | 1079 | | | -18.555 -19.847 | 17.357 | 1.00 16.40 |
| MOTA | 7318 | | 1079 | | | | | 1.00 15.90 |
| ATOM | 7319 | CB VAL | 1079 | | | -19.972 | 18.562 | 1.00 16.02 |
| MOTA | 7320 | CG1 VAL | 1079 1079 | | | -21.169 | 19.519 | 1.00 15.56 1.00 11.83 |
| ATOM . | | CG2 VAL | | | | -20.161 | 17.418 | |
| ATOM | 7322 | C VAL | 1079 | | | -19.977 | 19.163 19.971 | 1.00 18.15 1.00 20.36 |
| MOTA | 7323 7324 | O VAL | 1079 1080 | | | -19.056 -21.113 | 19.971 | 1.00 20.36 |
| MOTA MOTA | 7324 | N LEU CA LEU | 1080 | | | -21.113 | 20.296 | 1.00 20.11 |
| | 7325 | CB LEU | 1080 | | | -21.401 | 19.730 | 1:00 20.37 |
| ATOM | 7327 | CG LEU | 1080 | | | -20.659 | 19.730 | 1.00 21.80 |
| MOTA | | | 1080 | | | -21.278 | 18.936 | 1.00 24.33 |
| MOTA MOTA | 7328 7329 | CD1 LEU CD2 LEU | 1080 | | | -21.278 -19.794 | 20.637 | 1.00 22.66 |
| | 7330 | C LEU | 1080 | | | -22.584 | 21.085 | 1.00 23.33 |
| MOTA MOTA | 7331 | O LEU | 1080 | | | -23.659 | 20.526 | 1.00 19.20 |
| ATOM | 7331 | N GLU | 1080 | | | -23.039 | 22.379 | 1.00 20.64 |
| ATOM | 7332 | CA GLU | 1081 | | | -23.439 | 23.224 | 1.00 20.04 |
| ATOM | 7334 | CB GLU | 1081 | | | -22.988 | 23.790 | 1.00 21.33 |
| ATOM | 7335 | CG GLU | 1081 | | | -23.952 | 24.779 | 1.00 21.73 |
| ATOM | 7336 | CD GLU | 1081 | | | -23.532 | 25.073 | 1.00 25.66 |
| ATOM | 7337 | OE1 GLU | 1081 | | 18.223 | -22.519 | 24.712 | 1.00 24.72 |
| ATOM | 7338 | OE2 GLU | 1081 | | | -24.481 | 25.673 | 1.00 25.08 |
| ATOM | 7339 | C GLU | 1081 | | | -23.897 | 24.364 | 1.00 23.06 |
| MOTA | 7340 | O GLU | 1081 | | | -23.037 | 25.118 | 1.00 22.00 |
| ATOM | 7341 | N CYS | 1082 | | | -25.215 | 24.471 | 1.00 23.09 |
| ATOM | 7342 | CA CYS | 1082 | | | -25.861 | 25.503 | 1.00 23.95 |
| ATOM | 7343 | CB CYS | 1082 | | | -26.008 | 26.776 | 1.00 25.09 |
| | | | | | | | | |

| ATOM | 7344 | SG | CYS | 1082 | -21.655 | -26.980 | 26.505 | 1.00 27.14 |
|------|------|-----|-----|------|---------|---------|--------|------------|
| ATOM | 7345 | С | CYS | 1082 | -25.276 | -25.148 | 25.800 | 1.00 25.48 |
| ATOM | 7346 | 0 | CYS | 1082 | -25.409 | -24.431 | 26.795 | 1.00 25.29 |
| ATOM | 7347 | N | VAL | 1083 | | -25.372 | 24.915 | 1.00 26.92 |
| ATOM | 7348 | CA | VAL | 1083 | | -24.784 | 25.012 | 1.00 29.17 |
| ATOM | 7349 | CB | VAL | 1083 | -27.646 | | 24.129 | 1.00 28.96 |
| | | | | 1083 | | | | 1.00 20.30 |
| ATOM | 7350 | CG1 | | | | -23.900 | 22.655 | |
| MOTA | 7351 | CG2 | | 1083 | | -22.729 | 24.450 | 1.00 32.97 |
| MOTA | 7352 | С | VAL | 1083 | -28.559 | | 24.508 | 1.00 29.38 |
| ATOM | 7353 | 0 | VAL | 1083 | | -26.570 | 23.559 | 1.00 28.35 |
| MOTA | 7354 | N | PRO | 1084 | | -25.911 | 25.138 | 1.00 30.34 |
| ATOM | 7355 | CD | PRO | 1084 | -30.314 | -25.021 | 26.160 | 1.00 29.84 |
| ATOM | 7356 | CA | PRO | 1084 | -30.728 | -26.896 | 24.688 | 1.00 30.70 |
| ATOM | 7357 | СВ | PRO | 1084 | -31.989 | -26.510 | 25.471 | 1.00 30.48 |
| ATOM | 7358 | CG | PRO | 1084 | | -25.059 | 25.807 | 1.00 31.98 |
| ATOM | 7359 | С | PRO | 1084 | | -26.865 | 23.176 | 1.00 31.50 |
| ATOM | 7360 | ō | PRO | 1084 | | -25.794 | 22.572 | 1.00 32.64 |
| ATOM | 7361 | N | VAL | 1085 | | -28.049 | 22.574 | 1.00 32.04 |
| | | | | | | | | 1.00 32.04 |
| MOTA | 7362 | CA | VAL | 1085 | -31.157 | | 21.134 | |
| MOTA | 7363 | CB | VAL | 1085 | | -29.648 | 20.748 | 1.00 33.17 |
| MOTA | 7364 | | VAL | 1085 | -31.544 | | 19.239 | 1.00 32.51 |
| ATOM | 7365 | CG2 | | 1085 | -30.392 | | 21.309 | 1.00 32.67 |
| ATOM | 7366 | С | VAL | 1085 | -32.291 | -27.305 | 20.632 | 1.00 34.32 |
| ATOM | 7367 | 0 | VAL | 1085 | -32.224 | -26.755 | 19.530 | 1.00 33.11 |
| MOTA | 7368 | N | GLU | 1086 | -33.325 | -27.176 | 21.457 | 1.00 36.11 |
| ATOM | 7369 | CA | GLU | 1086 | -34.500 | -26.371 | 21.131 | 1.00 38.46 |
| ATOM | 7370 | СВ | GLU | 1086 | | -26.364 | 22.313 | 1.00 40.09 |
| ATOM | 7371 | CG | GLU | 1086 | | -27.605 | 23.195 | 1.00 42.70 |
| ATOM | 7372 | CD | GLU | 1086 | -35.426 | | 22.402 | 1.00 44.30 |
| | | | | | | | | |
| ATOM | 7373 | | GLU | 1086 | | -29.040 | | 1.00 45.21 |
| MOTA | 7374 | | GLU | 1086 | -34.626 | | 22.614 | 1.00 45.27 |
| ATOM | 7375 | С | GLU | 1086 | -34.097 | | 20.812 | 1.00 37.16 |
| MOTA | 7376 | 0 - | GLU | 1086 | -34.441 | -24.400 | 19.758 | 1.00 37.62 |
| ATOM | 7377 | N | LEU | 1087 | | -24.316 | 21.736 | 1.00 37.02 |
| MOTA | 7378 | CA | LEU | 1087 | -32.928 | -22.941 | 21.562 | 1.00 36.84 |
| ATOM | 7379 | CB | LEU | 1087 | -32.192 | -22.455 | 22.813 | 1.00 38.04 |
| ATOM | 7380 | CG | LEU | 1087 | -32.583 | -21.085 | 23.384 | 1.00 39.52 |
| ATOM | 7381 | | LEU | 1087 | | -20.804 | 24.630 | 1.00 40.56 |
| ATOM | 7382 | | LEU | 1087 | | -19.994 | 22.349 | 1.00 39.60 |
| | 7383 | C | LEU | 1087 | -32.020 | | 20.345 | 1.00 36.08 |
| ATOM | | | | | | | | 1.00 35.75 |
| MOTA | 7384 | 0 | LEU | 1087 | -32.141 | | 19.570 | |
| ATOM | 7385 | N | ALA | 1088 | -31.116 | | 20.173 | 1.00 35.37 |
| ATOM | 7386 | CA | ALA | 1088 | | -23.757 | 19.038 | 1.00 34.84 |
| ATOM | 7387 | CB | ALA | 1088 | | -24.989 | 19.066 | 1.00 32.98 |
| ATOM | 7388 | C | ALA | 1088 | | -23.700 | 17.722 | 1.00 35.07 |
| ATOM | 7389 | 0 | ALA | 1088 | -30.530 | -23.059 | 16.765 | 1.00 35.13 |
| ATOM | 7390 | N | LYS | 1089 | -32.112 | -24.372 | 17.685 | 1.00 36.00 |
| ATOM | 7391 | CA | LYS | 1089 | -32.952 | -24.402 | 16.493 | 1.00 37.51 |
| ATOM | 7392 | CB | LYS | 1089 | -34.133 | -25.353 | 16.702 | 1.00 40.32 |
| ATOM | 7393 | CG | LYS | 1089 | -33.741 | -26.772 | 17.054 | 1.00 42.81 |
| ATOM | 7394 | CD | LYS | 1089 | | -27.619 | 17.354 | 1.00 46.04 |
| | 7395 | CE | LYS | 1089 | -34.575 | | 17.818 | 1.00 46.35 |
| MOTA | | | | | | | | |
| MOTA | 7396 | NZ | LYS | 1089 | -35.755 | | 18.300 | 1.00 47.78 |
| MOTA | 7397 | С | LYS | 1089 | | -23.014 | 16.161 | 1.00 35.60 |
| MOTA | 7398 | 0 | LYS | 1089 | -33.330 | -22.536 | 15.039 | 1.00 35.12 |
| MOTA | 7399 | N | ARG | 1090 | -34.117 | -22.374 | 17.141 | 1.00 35.99 |
| MOTA | 7400 | CA | ARG | 1090 | -34.681 | -21.039 | 16.947 | 1.00 36.46 |
| MOTA | 7401 | CB | ARG | 1090 | -35.288 | -20.511 | 18.247 | 1.00 38.53 |
| MOTA | 7402 | CG | ARG | 1090 | -36.350 | -21.392 | 18.862 | 1.00 42.68 |
| ATOM | 7403 | CD | ARG | 1090 | -37.186 | -20.592 | 19.842 | 1.00 45.65 |
| MOTA | 7404 | NE | ÀRG | 1090 | -36.365 | -19.905 | 20.834 | 1.00 49.18 |
| MOTA | 7405 | CZ | ARG | 1090 | -36.842 | -19.046 | 21.730 | 1.00 50.27 |
| ATOM | 7406 | | ARG | 1090 | -38.137 | -18.769 | 21.758 | 1.00 51.07 |
| | | | | 1090 | -36.029 | -18.464 | 22.601 | 1.00 51.07 |
| ATOM | 7407 | | ARG | | | | | |
| MOTA | 7408 | С | ARG | 1090 | | -20.038 | 16.458 | 1.00 34.36 |
| MOTA | 7409 | 0 | ARG | 1090 | -33.859 | | 15.472 | 1.00 34.30 |
| MOTA | 7410 | N | ILE | 1091 | -32.513 | -19.976 | 17.163 | 1.00 32.94 |
| MOTA | 7411 | CA | ILE | 1091 | -31.432 | -19.059 | 16.820 | 1.00 30.49 |
| MOTA | 7412 | CB | ILE | 1091 | | -19.179 | 17.828 | 1.00 29.84 |
| ATOM | 7413 | CG2 | ILE | 1091 | -29.087 | -18.304 | 17.382 | 1.00 26.75 |
| ATOM | 7414 | | ILE | 1091 | -30.749 | -18.770 | 19.222 | 1.00 27.82 |
| ATOM | 7415 | | ILE | 1091 | -29.749 | | 20.332 | 1.00 28.01 |
| ATOM | 7416 | C | ILE | 1091 | -30.904 | | 15.418 | 1.00 29.96 |
| ATOM | 7417 | 0 | ILE | 1091 | | -18.374 | 14.650 | 1.00 30.26 |
| ATOM | 7418 | N | | 1092 | -30.711 | | 15.078 | 1.00 30.58 |
| | | | THR | | | | 13.760 | 1.00 30.38 |
| ATOM | 7419 | CA | THR | 1092 | | -20.929 | | |
| MOTA | 7420 | CB | THR | 1092 | -29.921 | -22.433 | 13.645 | 1.00 31.25 |
| | | | | | | | | |

| ATOM | 7421 | OG1 | THR | 1092 | -28.972 | -22.827 | 14.648 | 1.00 31.53 |
|--------------|--------------|---------|------------|--------------|--------------------|--------------------|------------------|--------------------------|
| ATOM | 7422 | CG2 | THR | 1092 | -29.357 | -22.760 | 12.269 | 1.00 29.03 |
| ATOM | 7423 | C | THR | 1092 | -31.156 | -20.527 | 12.654 | 1.00 31.78 |
| ATOM | 7424 | 0 | THR | 1092 | -30.742 | -20.039 | 11.602 | 1.00 32.76 |
| ATOM | 7425 | N | GLU | 1093 | -32.443 | -20.742 | 12.897 | 1.00 32.97 |
| ATOM | 7426 | CA | GLU | 1093 | -33.467 | -20.405 | 11.918 | 1.00 34.29 |
| MOTA | 7427 | CB | GLU | 1093 | -34.743 | -21.190 | 12.215 | 1.00 35.93 |
| ATOM | 7428 | CG | GLU | 1093 | -34.531 | -22.694 | 12.240 | 1.00 40.74 |
| MOTA | 7429 | CD | GLU | 1093 | -35.785 | -23.460 | 12.620 | 1.00 44.39 |
| MOTA | 7430 | OE1 | GLU | 1093 | -36.357 | -23.178 | 13.698 | 1.00 46.36 |
| MOTA | 7431 | OE2 | GLU | 1093 | -36.193 | -24.347 | 11.842 | 1.00 45.61 |
| MOTA | 7432 | С | GLU | 1093 | -33.760 | -18.909 | 11.913 | 1.00 32.84 |
| MOTA | 7433 | 0 | GLU | 1093 | -34.238 | -18.366 | 10.915 | 1.00 33.67 |
| ATOM | 7434 | N | ALA | 1094 | -33,461 | -18.244 | 13.024 | 1.00 32.28 |
| ATOM | 7435 | CA | ALA | 1094 | -33.705 | -16.810 | 13.138 | 1.00 30.66 |
| ATOM | 7436 | CB | ALA | 1094 | | -16.430 | 14.602 | 1.00 31.86 |
| ATOM | 7437 | С | ALA | 1094 | | -15.965 | 12.503 | 1.00 29.98 |
| MOTA | 7438 | 0 | ALA | 1094 | | -14.912 | 11.927 | 1.00 29.52 |
| ATOM | 7439 | N | LEU | 1095 | | -16.424 | 12.602 | 1.00 27.75 |
| ATOM | 7440 | CA | LEU | 1095 | | -15.677 | 12.035 | 1.00 26.60 |
| MOTA | 7441 | CB | LEU | 1095 | | -15.892 | 12.875 | 1.00 27.24 |
| MOTA | 7442 | CG | LEU | 1095 | | -15.409 | 14.327 | 1.00 28.91 |
| ATOM | 7443 | | LEU | 1095 | | -15.587 | 14.941 | 1.00 28.85 |
| ATOM | 7444 | | LEU | 1095 | | -13.948 | 14.386 | 1.00 32.53 |
| ATOM | 7445 | С | LEU | 1095 | | -16.024 | 10.581 | 1.00 25.13 |
| ATOM | 7446 | 0 | LEU | 1095 | | -17.176 | 10.161 | 1.00 25.13 |
| ATOM | 7447 | N | ALA | 1096 | | -15.016 | 9.813 | 1.00 23.38 |
| ATOM | 7448 | CA | ALA | 1096 | | -15.221 | 8.417 | 1.00 24.18 |
| ATOM | 7449 | CB | ALA | 1096 | | -13.921 | 7.636 | 1.00 26.66 |
| ATOM ATOM | 7450 7451 | С | ALA | 1096 | | -15.704 | 8.340 | 1.00 23.29 |
| | 7451 | O N | ALA | 1096 1097 | | -16.473 -15.253 | 7.446 9.278 | 1.00 22.71 1.00 22.57 |
| ATOM ATOM | 7453 | CA | ILE ILE | 1097 | | -15.662 | 9.276 | 1.00 22.02 |
| ATOM | 7454 | CB | ILE | 1097 | | -14.773 | 10.231 | 1.00 22.02 |
| MOTA | 7455 | | ILE | 1097 | | -13.339 | 9.735 | 1.00 20.50 |
| ATOM | 7456 | CG1 | | 1097 | | -14.868 | 11.671 | 1.00 19.11 |
| ATOM | 7457 | CD1 | | 1097 | | -14.180 | 12.681 | 1.00 15.11 |
| ATOM | 7458 | C | ILE | 1097 | | -17.099 | 9.779 | 1.00 21.40 |
| ATOM | 7459 | o | ILE | 1097 | | -17.594 | 10.489 | 1.00 20.96 |
| ATOM | 7460 | N | PRO | 1098 | | -17.793 | 9.391 | 1.00 21.86 |
| ATOM | 7461 | CD | PRO | 1098 | | -17.422 | 8.409 | 1.00 22.08 |
| ATOM | 7462 | CA | PRO | 1098 | | -19.180 | 9.832 | 1.00 22.32 |
| ATOM | 7463 | CB | PRO | 1098 | | -19.700 | 8.968 | 1.00 21.93 |
| ATOM | 7464 | CG | PRO | 1098 | | -18.469 | 8.626 | 1.00 24.68 |
| ATOM | 7465 | С | PRO | 1098 | -23.896 | -19.316 | 11.329 | 1.00 22.49 |
| ATOM | 7466 | 0 | PRO | 1098 | -23.160 | -18.528 | 11.933 | 1.00 21.97 |
| ATOM | 7467 | N | VAL | 1099 | -24.527 | -20.317 | 11.930 | 1.00 21.40 |
| ATOM | 7468 | CA | VAL | 1099 | -24.368 | -20.569 | 13.351 | 1.00 20.38 |
| ATOM | 7469 | CB | VAL | 1099 | -25.735 | -20.667 | 14.048 | 1.00 21.59 |
| MOTA | 7470 | CG1 | VAL | 1099 | -25.543 | -21.007 | 15.518 | 1.00 20.95 |
| MOTA | 7471 | | VAL | 1099 | -26.485 | -19.348 | 13.902 | 1.00 20.13 |
| ATOM | 7472 | С | VAL | | | -21.862 | 13.568 | 1.00 20.91 |
| ATOM | 7473 | 0 | VAL | 1099 | | -22.929 | 13.119 | 1.00 21.10 |
| ATOM | 7474 | N | ILE | 1100 | | -21.749 | 14.252 | 1.00 20.43 |
| MOTA | 7475 | CA | ILE | 1100 | | -22.897 | 14.553 | 1.00 19.39 |
| ATOM | 7476 | CB | ILE | 1100 | | -22.533 | 14.393 | 1.00 18.61 |
| ATOM | 7477 | CG2 | ILE | 1100 | | -23.709 | 14.814 | 1.00 21.73 |
| ATOM . | 7478 | CG1 | | 1100 | -19.807 | | 12.939 | 1.00 19.30 |
| ATOM | 7479 | | ILE | 1100 | -18.369 -21 862 | | 12.698 | 1.00 18.01 1.00 17.92 |
| MOTA | 7480 | C | ILE | 1100 | -21.862 | | 15.992 | |
| MOTA | 7481 7482 | O N | ILE GLY | 1100 1101 | | -22.541 -24.629 | 16.925 16.179 | 1.00 19.15 1.00 17.28 |
| MOTA | | | | | | | 17.521 | |
| ATOM ATOM | 7483 7484 | CA C | GLY GLY | 1101 1101 | | -25.087 -26.058 | 18.134 | 1.00 15.61 1.00 16.33 |
| ATOM | 7485 | o | GLY | 1101 | -20.607 | | 17.449 | 1.00 10.33 |
| ATOM | 7486 | N | ILE | 1101 | -21.450 | | 19.457 | 1.00 14.73 |
| ATOM | 7487 | CA | ILE | 1102 | -20.642 | | 20.228 | 1.00 17.43 |
| ATOM | 7488 | CB | ILE | 1102 | -19.213 | | 20.587 | 1.00 17.15 |
| ATOM | 7489 | | ILE | 1102 | -19.297 | | 21.214 | 1.00 16.29 |
| ATOM | 7490 | CG1 | | 1102 | -18.514 | | 21.519 | 1.00 17.38 |
| ATOM | 7491 | | ILE | 1102 | -17.048 | | 21.769 | 1.00 17.39 |
| ATOM | 7492 | C | ILE | 1102 | -21.486 | | 21.466 | 1.00 16.49 |
| ATOM | 7493 | ō | ILE | 1102 | -21.652 | | 22.324 | 1.00 18.86 |
| ATOM | 7494 | N | GLY | 1103 | -22.064 | | 21.525 | 1.00 18.98 |
| ATOM | 7495 | CA | GLY | 1103 | -22.913 | | 22.649 | 1.00 19.60 |
| ATOM | 7496 | C | GLY | 1103 | -24.275 | -28.209 | 22.470 | 1.00 21.48 |
| ATOM | 7497 | 0 | GLY | 1103 | -24.969 | -27.921 | 23.443 | 1.00 22.27 |
| | | | | | | | | |

| ATOM | 7498 | N | ALA | 1104 | -24.652 | -27.972 | 21.217 | 1.00 22.82 |
|-------|--------------|-----------|-----|------|---------|---------|--------|------------|
| ATOM | 7499 | CA | ALA | 1104 | -25.935 | -27.353 | 20.908 | 1.00 25.45 |
| ATOM | 7500 | CB | ALA | 1104 | -25.716 | -25.988 | 20.259 | 1.00 25.68 |
| MOTA | 7501 | C | ALA | 1104 | -26.771 | | 19.987 | 1.00 25.66 |
| ATOM | 7502 | ō | ALA | 1104 | -27.830 | | 19.515 | 1.00 26.77 |
| ATOM | 7503 | N | GLY | 1105 | -26.293 | | 19.722 | 1.00 26.62 |
| | 7504 | CA | GLY | 1105 | -27.026 | | 18.852 | 1.00 26.39 |
| ATOM | | | | | | | 17.400 | 1.00 26.35 |
| MOTA | 7505 | C | GLY | 1105 | -26.597 | | | |
| MOTA | 7506 | 0 | GLY | 1105 | -25.665 | | 17.087 | 1.00 27.27 |
| MOTA | 7507 | N | ASN | 1106 | -27.276 | | 16.514 | 1.00 24.67 |
| MOTA | 7508 | CA | ASN | 1106 | -26.946 | | 15.095 | 1.00 25.28 |
| MOTA | 7509 | CB | ASN | 1106 | -27.003 | | 14.513 | 1.00 27.03 |
| ATOM | 7510 | CG | ASN | 1106 | -28.406 | | 14.543 | 1.00 28.79 |
| MOTA | 7511 | OD1 | ASN | 1106 | -28.706 | | 13.810 | 1.00 30.36 |
| ATOM | 7512 | ND2 | ASN | 1106 | -29.267 | -32.414 | 15.398 | 1.00 26.73 |
| ATOM | 7513 | С | ASN | 1106 | -27.851 | -30.036 | 14.273 | 1.00 25.16 |
| ATOM | 7514 | 0 | ASN | 1106 | -27.889 | -30.133 | 13.046 | 1.00 26.21 |
| MOTA | 7515 | N | VAL | 1107 | -28.563 | -29.143 | 14.949 | 1.00 26.94 |
| ATOM | 7516 | CA | VAL | 1107 | -29.476 | | 14.287 | 1.00 27.66 |
| ATOM | 7517 | CB | VAL | 1107 | -30.583 | | 15.255 | 1.00 29.34 |
| ATOM | 7518 | | VAL | 1107 | -31.608 | | 14.507 | 1.00 33.27 |
| ATOM | 7519 | | VAL | 1107 | -31.250 | | 15.898 | 1.00 30.08 |
| | 7520 | | | 1107 | -28.751 | | 13.761 | 1.00 27.29 |
| ATOM | | C | VAL | | -29.274 | | 12.915 | 1.00 27.23 |
| ATOM | 7521 | 0 | VAL | 1107 | | | | |
| ATOM | 7522 | N | THR | 1108 | -27.547 | | 14.267 | 1.00 24.64 |
| ATOM | 7523 | CA | THR | 1108 | -26.769 | | 13.840 | 1.00 22.37 |
| MOTA | 7524 | CB | THR | 1108 | -25.594 | | 14.805 | 1.00 21.49 |
| ATOM | 7525 | OG1 | THR | 1108 | -24.814 | -26.532 | 14.944 | 1.00-20.03 |
| ATOM | 7526 | CG2 | THR | 1108 | -26.116 | -24.918 | 16.171 | 1.00 20.67 |
| ATOM | 7527 | С | THR | 1108 | -26.242 | -25.787 | 12.424 | 1.00 22.32 |
| ATOM | 7528 | 0 | THR | 1108 | -26.276 | -26.891 | 11.888 | 1.00 23.83 |
| MOTA | 7529 | N | ASP | 1109 | -25.764 | -24.705 | 11.820 | 1.00 21.15 |
| ATOM | 7530 | CA | ASP | 1109 | -25.241 | -24.746 | 10.461 | 1.00 21.07 |
| ATOM | 7531 | ĊB | ASP | 1109 | -25.122 | | 9.918 | 1.00 22.92 |
| ATOM | 7532 | CG | ASP | 1109 | -26.450 | | 9.904 | 1.00 25.19 |
| ATOM | 7533 | | ASP | 1109 | -27.371 | | 9.220 | 1.00 22.36 |
| | 7534 | | | 1109 | -26.577 | | 10.589 | 1.00 26.54 |
| MOTA | | | ASP | | -23.889 | | 10.389 | 1.00 20.97 |
| MOTA | 7535 | C | ASP | 1109 | | | | |
| MOTA | 7536 | 0 | ASP | 1109 | -23.511 | | 9.353 | |
| MOTA | 7537 | N | GLY | 1110 | -23.161 | | 11.498 | 1.00 21.29 |
| MOTA | 7538 | CA | GLY | 1110 | -21.855 | | 11.541 | 1.00 19.83 |
| ATOM | 7539 | С | GLY | 1110 | -21.532 | | 12.920 | 1.00 18.45 |
| MOTA | 7540 | Ö | GLY | 1110 | | -26.421 | 13.856 | 1.00 16.61 |
| ATOM | 7541 | N | GLN | 1111 | | -27.169 | 13.046 | 1.00 18.75 |
| ATOM | 7542 | CA | GLN | 1111 | -19.920 | -27.725 | 14.315 | 1.00 18.97 |
| ATOM | 7543 | CB | GLN | 1111 | -20.030 | -29.253 | 14.300 | 1.00 20.40 |
| ATOM | 7544 | CG | GLN | 1111 | -21.434 | -29.822 | 14.149 | 1.00 21.52 |
| ATOM | 7545 | CD | GLN | 1111 | -22.353 | -29.426 | 15.281 | 1.00 22.47 |
| ATOM | 7546 | | GLN | 1111 | -21.950 | -29.393 | 16.448 | 1.00 25.39 |
| ATOM | 7547 | NE2 | | 1111 | -23.607 | | 14.946 | 1.00 23.89 |
| ATOM | 7548 | C | GLN | 1111 | -18.462 | | 14.596 | 1.00 17.61 |
| ATOM | 7549 | 0 | GLN | 1111 | -17.697 | | 13.679 | 1.00 16.60 |
| | 7550 | | | 1112 | -18.089 | | 15.871 | 1.00 17.79 |
| ATOM. | | N | ILE | | -16.716 | | 16.276 | 1.00 17.75 |
| ATOM | 7551 | CA | ILE | 1112 | | | 16.531 | 1.00 18.72 |
| MOTA | 7552 | CB | ILE | 1112 | -16.454 | | | |
| ATOM | 7553 | CG2 | ILE | 1112 | -17.191 | | 17.786 | 1.00 18.50 |
| MOTA | 7554 | CG1 | | 1112 | -14.945 | | 16.671 | 1.00 18.93 |
| ATOM | 7555 | CD1 | | 1112 | | -23.906 | 16.715 | 1.00 20.59 |
| ATOM | 7556 | C | ILE | 1112 | -16.417 | -27.941 | 17.540 | 1.00 21.11 |
| MOTA | 7557 | 0 | ILE | 1112 | -17.319 | -28.264 | 18.321 | 1.00 20.41 |
| ATOM | 7558 | N | LEU | 1113 | -15.148 | -28.288 | 17.720 | 1.00 22.35 |
| MOTA | 7559 | CA | LEU | 1113 | -14.726 | -29.054 | 18.880 | 1.00 23.98 |
| ATOM | 7560 | CB | LEU | 1113 | -15.130 | -30.515 | 18.700 | 1.00 28.74 |
| ATOM | 7561 | CG | LEU | 1113 | -15.427 | -31.304 | 19.980 | 1.00 32.72 |
| MOTA | 7562 | | LEU | 1113 | -16.778 | -30.878 | 20.556 | 1.00 32.53 |
| ATOM | 7563 | CD2 | | 1113 | -15.441 | -32.784 | 19.648 | 1.00 35.33 |
| ATOM | 7564 | C | LEU | 1113 | -13.212 | -28.947 | 18.990 | 1.00 23.34 |
| | 7565 | o | LEU | 1113 | -12.534 | -28.716 | 17.983 | 1.00 22.61 |
| ATOM | 7566 | N | VAL | 1114 | -12.687 | -29.104 | 20.205 | 1.00 21.36 |
| | | | VAL | 1114 | -11.246 | -29.044 | 20.440 | 1.00 19.62 |
| MOTA | 7567 7569 | CA | | | | -28.996 | 21.966 | 1.00 19.02 |
| ATOM | 7568 7560 | CB CC1 | VAL | 1114 | | -28.834 | 22.187 | 1.00 20.48 |
| MOTA | 7569 | CG1 | | 1114 | | | | |
| ATOM | 7570 | | VAL | 1114 | | -27.870 | 22.620 | 1.00 20.82 |
| ATOM | 7571 | С | VAL | 1114 | | -30.304 | 19.851 | 1.00 18.23 |
| ATOM | 7572 | 0 | VAL | 1114 | -11.017 | | 20.210 | 1.00 18.70 |
| MOTA | 7573 | N | MET | 1115 | | -30.137 | 18.943 | 1.00 16.13 |
| MOTA | 7574 | CA | MET | 1115 | -9.041 | -31.287 | 18.305 | 1.00 14.70 |

| MOTA | 7575 | CB | MET | 1115 | -7.900 | -30.830 | 17.390 | 1.00 14.14 |
|--------------|--------------|-----------|------------|---------------------|---------|--------------------|------------------|--------------------------|
| ATOM | 7576 | CG | MET | 1115 | -6.823 | -30.025 | 18.095 | 1.00 15.65 |
| MOTA | 7577 | SD | MET | 1115 | -5.242 | -30.356 | 17.297 | 1.00 13.45 |
| ATOM | 7578 | CE | MET | 1115 | -4.722 | -31.861 | 18.197 | 1.00 11.23 |
| MOTA | 7579 | С | MET | 1115 | -8.492 | -32.315 | 19.287 | 1.00 13.25 |
| MOTA | 7580 | 0 | MET | 1115 | | -33.510 | 19.019 | 1.00 16.95 |
| MOTA | 7581 | N | HIS | 1116 | | -31.866 | 20.421 | 1.00 12.84 |
| MOTA | 7582 | CA | HIS | 1116 | -7.414 | -32.828 | 21.377 | 1.00 14.12 |
| MOTA | 7583 | CB | HIS | 1116 | | -32.107 | 22.521 | 1.00 13.42 |
| MOTA | 7584 | CG | HIS | 1116 | | -31.336 | 22.084 | 1.00 14.34 |
| MOTA | 7585 | | HIS | 1116 | | -30.121 | 21.494 | 1.00 12.56 |
| MOTA | 7586 | | HIS | 1116 | | -31.839 | 22.165 | 1.00 14.51 |
| MOTA | 7587 | | HIS | 1116 | | -30.971 | 21.646 | 1.00 12.60 |
| MOTA | 7588 | | HIS | 1116 | | -29.919 | 21.230 | 1.00 19.44 |
| MOTA | 7589 | C | HIS | 1116 | | -33.784 | 21.920 | 1.00 14.04 |
| ATOM | 7590 | 0 | HIS | 1116 | | -34.939 | 22.232 | 1.00 16.57 |
| ATOM | 7591 | N | ASP | 1117 | | -33.318 | 22.041 | 1.00 12.82 |
| ATOM | 7592 | CA | ASP | 1117 | | -34.176 | 22.536 | 1.00 15.57 |
| ATOM | 7593 | CB | ASP | 1117 | | -33.359 | 22.984 | 1.00 15.67 |
| ATOM | 7594 | CG | ASP | 1117 | | -32.484 | 24.179 | 1.00 15.82 |
| ATOM | 7595 | | ASP | 1117 | | -32.772 | 24.947 | 1.00 15.40 1.00 16.01 |
| ATOM | 7596 | | ASP | 1117 | | -31.500 | 24.364 | 1.00 16.01 1.00 17.95 |
| MOTA | 7597 7598 | C | ASP ASP | 1117 1117 | | -35.108 -36.306 | 21.424 21.633 | 1.00 17.93 |
| MOTA | 7599 | N O | ALA | 1118 | | -34.533 | 20.237 | 1.00 18.76 |
| MOTA | 7600 | | ALA | 1118 | | -35.267 | 19.073 | 1.00 20.93 |
| ATOM ATOM | 7601 | CA CB | ALA | 1118 | | -34.286 | 17.965 | 1.00 20.95 |
| ATOM | 7602 | C | ALA | 1118 | | -34.200 | 18.525 | 1.00 21.33 |
| ATOM | 7602 | 0 | ALA | 1118 | | -37.225 | 17.815 | 1.00 23.45 |
| ATOM | 7604 | N | PHE | 1119 | | -36.218 | 18.846 | 1.00 23.43 |
| MOTA | 7605 | CA | PHE | 1119 | | -37.179 | 18.340 | 1.00 27.36 |
| ATOM | 7606 | CB | PHE | 1119 | | -36.470 | 17.521 | 1.00 32.16 |
| ATOM | 7607 | CG | PHE | 1119 | | -35.714 | 16.375 | 1.00 35.71 |
| ATOM | 7608 | | PHE | 1119 | | -36.337 | 15.474 | 1.00 37.69 |
| ATOM | 7609 | | PHE | 1119 | | -34.371 | 16.203 | 1.00 38.44 |
| ATOM | 7610 | CE1 | | 1119 | | -35.633 | 14.420 | 1.00 40.51 |
| ATOM | 7611 | CE2 | | 1119 | | -33.660 | 15.152 | 1.00 39.76 |
| ATOM | 7612 | CZ | PHE | 1119 | | -34.287 | 14.256 | 1.00 41.23 |
| ATOM | 7613 | С | PHE | 1119 | -8.086 | -38.050 | 19.379 | 1.00 26.58 |
| MOTA | 7614 | О | PHE | 1119 | -6.942 | -38.460 | 19.212 | 1.00 30.89 |
| ATOM | 7615 | N | GLY | 1120 | -8.817 | -38.318 | 20.454 | 1.00 24.48 |
| ATOM | 7616 | CA | GLY | 1120 | -8.327 | -39.186 | 21.505 | 1.00 24.13 |
| MOTA | 7617 | C | GLY | 1120 | -7.005 | -38.851 | 22.160 | 1.00 23.63 |
| ATOM | 7618 | О | GLY | 1120 | | -39.758 | 22.581 | 1.00 22.16 |
| ATOM | 7619 | N | ILE | 1121 | -6.680 | -37.565 | 22.252 | 1.00 20.46 |
| MOTA | 7620 | CA | ILE | 1121 | | -37.145 | 22.900 | 1.00 19.00 |
| MOTA | 7621 | CB | ILE | 1121 | | -35.889 | 22.225 | 1.00 16.75 |
| ATOM | 7622 | CG2 | | 1121 | | -35.423 | 22.995 | 1.00 16.32 |
| ATOM | 7623 | CG1 | | 1121 | | -36.203 | 20.777 | 1.00 15.62 |
| ATOM | 7624 | CD1 | | 1121 | | -34.960 | 19.921 | 1.00 14.00 |
| ATOM | 7625 | С | ILE | 1121 | | -36.832 | 24.359 | 1.00 19.57 |
| ATOM | 7626 | 0 | ILE | 1121 | | -37.335 | 25.265 | 1.00 17.67 |
| ATOM | 7627 | N | THR | 1122 | | -36.009 | 24.591 | 1.00 20.23 |
| ATOM | 7628 | CA | THR | 1122 | | -35.671 | 25.958 | 1.00 23.81 |
| ATOM | 7629 7630 | CB OC1 | THR THR | 1122 1122 | | -34.773 -35.373 | 25.979 25.195 | 1.00 24.49 1.00 28.23 |
| ATOM | | | | | | | | |
| ATOM ATOM | 7631 7632 | CG2 | THR THR | $\frac{1122}{1122}$ | | -33.409 -36.940 | 25.402 26.751 | 1.00 18.95 1.00 26.71 |
| ATOM | 7632 | 0 | THR | 1122 | | -37.872 | 26.228 | 1.00 26.64 |
| ATOM | 7634 | N | GLY | 1123 | | -36.962 | 28.005 | 1.00 30.43 |
| ATOM | 7635 | CA | GLY | 1123 | | -38.113 | 28.870 | 1.00 37.27 |
| ATOM | 7636 | C | GLY | 1123 | | -39.059 | 28.484 | 1.00 39.65 |
| ATOM | 7637 | ō | GLY | 1123 | | -39.847 | 27.544 | 1.00 41.64 |
| ATOM | 7638 | N | GLY | 1124 | | -38.986 | 29.211 | 1.00 40.46 |
| ATOM | 7639 | CA | GLY | 1124 | | -39.852 | 28.920 | 1.00 38.97 |
| ATOM | 7640 | C | GLY | 1124 | | -39.208 | 29.340 | 1.00 37.18 |
| ATOM | 7641 | ō | GLY | 1124 | | -39.759 | 29.128 | 1.00 38.03 |
| ATOM | 7642 | N | HIS | 1125 | | -38.026 | 29.932 | 1.00 36.46 |
| ATOM | 7643 | CA | HIS | 1125 | | -37.290 | 30.399 | 1.00 35.97 |
| ATOM | 7644 | СВ | HIS | 1125 | | -36.726 | 31.792 | 1.00 37.38 |
| ATOM | 7645 | CG | HIS | 1125 | -12.325 | -37.771 | 32.812 | 1.00 39.81 |
| ATOM | 7646 | | HIS | 1125 | | -37.973 | 33.554 | 1.00 40.42 |
| ATOM | 7647 | ND1 | HIS | 1125 | -13.207 | -38.769 | 33.164 | 1.00 40.29 |
| ATOM | 7648 | | HIS | 1125 | | -39.541 | 34.081 | 1.00 40.40 |
| ATOM | 7649 | | HIS | 1125 | | -39.080 | 34.335 | 1.00 41.75 |
| MOTA | 7650 | С | HIS | 1125 | | -36.152 | 29.456 | 1.00 34.78 |
| MOTA | 7651 | 0 | HIS | 1125 | -13.410 | -35.000 | 29.880 | 1.00 36.44 |

| ATOM | 7652 | N | ILE | 1126 | -13.466 | -36.466 | 28.178 | 1.00 | 31.25 |
|--------------|--------------|------------|------------|--------------|--------------------|--------------------|------------------|------|----------------|
| MOTA | 7653 | CA | ILE | 1126 | | -35.435 | 27.215 | | 28.48 |
| ATOM | 7654 | CB | ILE | 1126 | -13.804 | -35.963 -36.360 | 25.767 | | 26.91 |
| ATOM ATOM | 7655 7656 | CG2 CG1 | ILE ILE | 1126 1126 | -12.394 -14.768 | -37.138 | 25.388 25.614 | | 26.98 25.19 |
| ATOM | 7657 | CD1 | ILE | 1126 | | -37.612 | 24.194 | | 22.08 |
| ATOM | 7658 | С | ILE | 1126 | | -34.961 | 27.540 | 1.00 | 28.29 |
| MOTA | 7659 | 0 | ILE | 1126 | | -35.702 | 28.122 | | 27.48 |
| MOTA | 7660 | N | PRO | 1127 | | -33.719 | 27.168 | | 27.02 |
| MOTA | 7661 7662 | CD CA | PRO PRO | 1127 1127 | | -32.750 -33.232 | 26.350 27.470 | | 26.06 27.27 |
| ATOM ATOM | 7663 | CB | PRO | 1127 | | -31.831 | 26.853 | 1.00 | 27.40 |
| ATOM | 7664 | CG | PRO | 1127 | | -31.927 | 25.749 | | 29.05 |
| ATOM | 7665 | С | PRO | 1127 | | -34.136 | 26.925 | | 27.42 |
| MOTA | 7666 | 0 | PRO | 1127 | | -34.877 | 25.962 | | 25.23 |
| ATOM | 7667 7668 | N CA | LYS LYS | 1128 1128 | | -34.081 -34.895 | 27.559 27.145 | | 28.67 29.40 |
| ATOM ATOM | 7669 | CB | LYS | 1128 | | -34.609 | 28.033 | | 32.06 |
| ATOM | 7670 | CG | LYS | 1128 | | -35.326 | 29.376 | | 37.86 |
| MOTA | 7671 | CD | LYS | 1128 | | -34.884 | 30.254 | | 41.77 |
| MOTA | 7672 | CE | LYS | 1128 | | -35.614 | 31.586 | | 42.92 |
| MOTA | 7673 | NZ | LYS | 1128 | -19.313 | -35.170 | 32.465 | | 45.73 28.13 |
| ATOM ATOM | 7674 7675 | C 0 | LYS LYS | 1128 1128 | | -34.674 -35.595 | 25.691 25.020 | | 28.71 |
| MOTA | 7676 | N | PHE | 1129 | -20.549 | | 25.208 | | 25.91 |
| MOTA | 7677 | CA | PHE | 1129 | -20.902 | -33.098 | 23.834 | 1.00 | 24.94 |
| MOTA | 7678 | CB | PHE | 1129 | -21.220 | | 23.761 | | 24.88 |
| ATOM | 7679 | CG | PHE | 1129 | -20.113 | | 24.268 | | 25.53 |
| ATOM ATOM | 7680 7681 | | PHE PHE | 1129 1129 | | -30.501 -30.098 | 23.508 25.508 | | 25.50 26.10 |
| ATOM | 7682 | | PHE | 1129 | | -29.678 | 23.976 | | 24.44 |
| ATOM | 7683 | | PHE | 1129 | -19.196 | | 25.989 | | 28.35 |
| MOTA | 7684 | CZ | PHE | 1129 | | -29.062 | 25.219 | | 25.02 |
| ATOM | 7685 | C | PHE | 1129 | | -33.444 | 22.809 | | 24.51 |
| ATOM ATOM | 7686 7687 | O N | PHE ALA | 1129 1130 | -20.017 -18.711 | -33.241 | 21.608 23.285 | | 25.21 22.79 |
| ATOM | 7688 | CA | ALA | 1130 | | -34.322 | 22.400 | | 22.40 |
| MOTA | 7689 | СВ | ALA | 1130 | | -33.933 | 23.047 | | 22.61 |
| MOTA | 7690 | С | ALA | 1130 | -17.587 | -35.793 | 22.030 | | 22.33 |
| ATOM ATOM | 7691 7692 | O N | ALA LYS | 1130 1131 | -18.222 -16.824 | -36.627 -36.105 | 22.674 20.992 | | 23.47 21.42 |
| ATOM | 7693 | CA | LYS | 1131 | | -37.473 | 20.534 | | 21.42 |
| ATOM | 7694 | CB | LYS | 1131 | | -37.723 | 19.374 | 1.00 | |
| MOTA | 7695 | CG | LYS | 1131 | -17.613 | -39.131 | 18.807 | | 25.99 |
| MOTA | 7696 | CD | LYS | 1131 | | -39.339 | 17.722 | | 27.36 |
| ATOM ATOM | 7697 7698 | CE NZ | LYS LYS | 1131 1131 | -18.521 -19.590 | -40.719 -41.000 | 17.096 16.100 | | 28.45 30.79 |
| ATOM | 7699 | C | LYS | 1131 | -15.272 | -37.770 | 20.099 | | 20.50 |
| ATOM | 7700 | Ō | LYS | 1131 | | -36.946 | 19.456 | 1.00 | 19.85 |
| ATOM | 7701 | N | ASN | 1132 | | -38.946 | 20.475 | 1.00 | 18.18 |
| ATOM | 7702 | CA | ASN | 1132 | | -39.373 | 20.100 | | 19.09 |
| ATOM ATOM | 7703 7704 | CB CG | ASN ASN | 1132 1132 | -12.860 | -40.286 | 21.178 20.775 | | 18.83 18.02 |
| ATOM | 7705 | OD1 | | 1132 | -11.079 | | 19.642 | | 17.99 |
| ATOM | 7706 | ND2 | ASN | 1132 | | -41.557 | 21.696 | 1.00 | 17.64 |
| MOTA | 7707 | С | ASN | 1132 | -13.563 | -40.141 | 18.786 | 1.00 | 18.64 |
| ATOM | 7708 | 0 | ASN | 1132 | | -41.332 | 18.781 | 1.00 | 19.00 |
| ATOM ATOM | 7709 7710 | N CA | PHE PHE | 1133 1133 | -13.296 -13.376 | -39.460 -40.079 | 17.678 16.361 | 1.00 | 18.32 18.77 |
| ATOM | 7711 | CB | PHE | 1133 | | -39.008 | 15.268 | 1.00 | 19.12 |
| MOTA | 7712 | CG | PHE | 1133 | -14.774 | -38.242 | 15.297 | 1.00 | 19.88 |
| MOTA | 7713 | | PHE | 1133 | | -37.142 | 16.127 | | 20.42 |
| ATOM | 7714 | CD2 | | 1133 | -15.858 -16.144 | -38.656 | 14.531 | 1.00 | 21.73 |
| ATOM ATOM | 7715 7716 | CE1 CE2 | PHE | 1133 1133 | | -36.453 -37.978 | 16.200 14.592 | | 22.46 |
| ATOM | 7717 | CZ | PHE | 1133 | | -36.879 | 15.431 | | 21.23 |
| MOTA | 7718 | С | PHE | 1133 | -12.208 | -40.999 | 16.036 | 1.00 | 18.83 |
| MOTA | 7719 | 0 | PHE | 1133 | -12.314 | | 15.144 | 1.00 | 19.05 |
| ATOM ATOM | 7720 7721 | N Ca | LEU | 1134 | -11.094 -9.920 | -40.849 -41.686 | 16.749 16.488 | 1.00 | 17.75 18.27 |
| ATOM ATOM | 7721 7722 | CA CB | LEU | 1134 1134 | | -41.086 | 17.230 | 1.00 | 17.93 |
| ATOM | 7723 | CG | LEU | 1134 | | -41.958 | 17.089 | 1.00 | 19.52 |
| MOTA | 7724 | CD1 | LEU | 1134 | -6.983 | -41.987 | 15.625 | 1.00 | 18.91 |
| ATOM | 7725 | | LEU | 1134 | | -41.335 | 17.936 | 1.00 | 16.96 |
| ATOM ATOM | 7726 | C | LEU | 1134 | | -43.126 -44.059 | 16.908 16.167 | 1.00 | 19.68 17.88 |
| ATOM | 7727 7728 | O N | LEU ALA | 1134 1135 | -10.727 | | 18.101 | | 22.36 |
| | 0 | | | | | - | | | |

| MOTA | 7729 | CA | ALA | 1135 | -11.027 | -44.623 | 18.617 | 1.00 27.76 |
|--------------|--------------|----------|------------|--------------|---------|--------------------|----------------|--------------------------|
| ATOM | 7730 | CB | ALA | 1135 | -11.775 | -44.513 | 19.934 | 1.00 26.50 |
| ATOM | 7731 | C | ALA | 1135 | -11.867 | -45.387 | 17.603 | 1.00 32.49 |
| ATOM | 7732 | 0 | ALA | 1135 | -11.683 | -46.590 | 17.403 | 1.00 33.61 |
| ATOM | 7733 | N | GLU | 1136 | -12.785 | -44.668 | 16.964 | 1.00 36.50 |
| MOTA | 7734 | CA | GLU | 1136 | -13.676 | -45.240 | 15.963 | 1.00 40.36 |
| ATOM | 7735 | CB | GLU | 1136 | -14.606 | -44.158 | 15.403 | 1.00 43.73 |
| ATOM | 7736 | CG | GLU | 1136 | | -43.403 | 16.441 | 1.00 48.10 |
| ATOM | 7737 | CD | GLU | 1136 | -16.536 | | 17.054 | 1.00 50.51 |
| ATOM | 7738 | OE1 | | 1136 | -16.222 | | 17.846 | 1.00 51.66 |
| ATOM | 7739 | | GLU | 1136 | -17.719 | | 16.735 | 1.00 51.42 |
| ATOM | 7740 | C | GLU | 1136 | -12.865 | | 14.820 | 1.00 41.02 |
| ATOM | 7741 | ō | GLU | 1136 | -12.942 | | 14.544 | 1.00 42.71 |
| ATOM | 7742 | N | THR | 1137 | | -44.979 | 14.155 | 1.00 39.55 |
| ATOM | 7743 | CA | THR | 1137 | | -45.406 | 13.033 | 1.00 38.43 |
| ATOM | 7744 | CB | THR | 1137 | -10.911 | | 12.124 | 1.00 39.66 |
| ATOM | 7745 | | THR | 1137 | | -44.569 | 11.313 | 1.00 41.87 |
| ATOM | 7746 | CG2 | THR | 1137 | -10.595 | | 12.953 | 1.00 37.36 |
| ATOM | 7747 | C | THR | 1137 | | -46.105 | 13.474 | 1.00 37.92 |
| ATOM | 7748 | ō | THR | 1137 | | -47.326 | 13.641 | 1.00 40.29 |
| ATOM | 7749 | N | GLY | 1138 | | -45.333 | 13.659 | 1.00 33.87 |
| ATOM | 7750 | CA | GLY | 1138 | | -45.905 | 14.084 | 1.00 31.20 |
| ATOM | 7751 | C | GLY | 1138 | | -45.066 | 13.574 | 1.00 29.12 |
| ATOM | 7752 | ō | GLY | 1138 | | -45.257 | 13.951 | 1.00 27.41 |
| ATOM | 7753 | N | ASP | 1139 | | -44.119 | 12.711 | 1.00 25.34 |
| ATOM | 7754 | CA | ASP | 1139 | | -43.224 | 12.105 | 1.00 23.78 |
| MOTA | 7755 | СВ | ASP | 1139 | | -43.614 | 10.635 | 1.00 27.59 |
| ATOM | 7756 | CG | ASP | | | -42.595 | 9.841 | 1.00 30.02 |
| ATOM | 7757 | | ASP | 1139 | | -41.880 | 9.048 | 1.00 26.93 |
| ATOM | 7758 | | ASP | 1139 | | -42.508 | 10.021 | 1.00 33.99 |
| ATOM | 7759 | C | ASP | 1139 | | -41.781 | 12.260 | 1.00 19.81 |
| ATOM | 7760 | ō | ASP | 1139 | | -41.536 | 12.137 | 1.00 17.74 |
| ATOM | 7761 | N | ILE | 1140 | -5.505 | -40.832 | 12.548 | 1.00 18.99 |
| ATOM | 7762 | CA | ILE | 1140 | -5.937 | -39.445 | 12.737 | 1.00 16.56 |
| MOTA | 7763 | CB | ILE | 1140 | -4.777 | -38.540 | 13.260 | 1.00 15.40 |
| ATOM | 7764 | CG2 | ILE | 1140 | -5.216 | -37.074 | 13.303 | 1.00 14.63 |
| MOTA | 7765 | CG1 | ILE | 1140 | -4.378 | -38.987 | 14.673 | 1.00 14.66 |
| ATOM | 7766 | CD1 | ILE | 1140 | | -38.193 | 15.276 | 1.00 14.86 |
| ATOM | 7767 | C | ILE | 1140 | | -38.792 | 11.507 | 1.00 15.51 |
| MOTA | 7768 | 0 | ILE | 1140 | | -38.099 | 11.627 | 1.00 15.94 |
| ATOM | 7769 | N | ARG | 1141 | | -39.003 | 10.325 | 1.00 15.97 |
| MOTA | 7770 | CA | ARG | 1141 | | -38.411 | 9.129 | 1.00 17.73 |
| ATOM | 7771 | CB | ARG | 1141 | | -38.608 | 7.916 | 1.00 18.46 |
| MOTA | 7772 | CG | ARG | 1141 | | -37.682 | 7.944 | 1.00 20.14 |
| ATOM | 7773 | CD | ARG | 1141 | | -37.933 | 6.816 | 1.00 19.99 |
| ATOM | 7774 | NE | ARG | 1141 | | -36.984 | 6.875 | 1.00 21.20 |
| ATOM | 7775 | CZ | ARG | 1141 | | -36.945 -37.805 | 7.843 | 1.00 21.99 1.00 20.45 |
| ATOM | 7776 | NH1 | | 1141 | | -36.042 | 8.851 7.804 | 1.00 20.45 |
| ATOM · | 7777 7778 | NH2 C | | 1141 1141 | | -39.026 | 8.885 | 1.00 23.21 |
| ATOM ATOM | 7779 | 0 | ARG ARG | 1141 | | -38.330 | 8.484 | 1.00 17.00 |
| ATOM | 7780 | N | ALA | 1141 | | -40.325 | 9.146 | 1.00 10.30 |
| ATOM | 7781 | CA | ALA | 1142 | | -41.004 | 8.963 | 1.00 17.72 |
| ATOM | 7782 | CB | ALA | 1142 | | -42.515 | 9.140 | 1.00 17.43 |
| ATOM | 7783 | C | ALA | 1142 | | -40.471 | 9.962 | 1.00 19.39 |
| ATOM | 7784 | 0 | ALA | 1142 | | -40.372 | 9.663 | 1.00 18.01 |
| ATOM | 7785 | N | ALA | 1143 | | -40.132 | 11.158 | 1.00 17.42 |
| ATOM | 7786 | CA | ALA | 1143 | | -39.600 | 12.177 | 1.00 18.14 |
| ATOM | 7787 | СВ | ALA | 1143 | | -39.468 | 13.510 | 1.00 17.85 |
| ATOM | 7788 | С | ALA | 1143 | | -38.240 | 11.716 | 1.00 16.90 |
| ATOM | 7789 | 0 | ALA | 1143 | -12.525 | -37.921 | 11.900 | 1.00 16.07 |
| MOTA | 7790 | N | VAL | 1144 | -10.464 | -37.449 | 11.115 | 1.00 16.80 |
| MOTA | 7791 | CA | VAL | 1144 | -10.826 | -36.135 | 10.603 | 1.00 17.64 |
| MOTA | 7792 | CB | VAL | 1144 | -9.604 | -35.412 | 9.989 | 1.00 17.57 |
| MOTA | 7793 | CG1 | VAL | 1144 | -10.050 | -34.114 | 9.326 | 1.00 15.63 |
| MOTA | 7794 | CG2 | VAL | 1144 | | -35.116 | 11.078 | 1.00 15.39 |
| ATOM | 7795 | С | VAL | 1144 | | -36.290 | 9.528 | 1.00 18.77 |
| MOTA | 7796 | 0 | VAL | 1144 | | -35.615 | 9.560 | 1.00 17.83 |
| ATOM | 7797 | N | ARG | 1145 | | -37.181 | 8.575 | 1.00 19.43 |
| ATOM | 7798 | CA | ARG | 1145 | | -37.408 | 7.507 | 1.00 21.72 |
| MOTA | 7799 | CB | ARG | 1145 | | -38.435 | 6.514 | 1.00 22.86 |
| ATOM | 7800 | CG | ARG | 1145 | | -37.920 | 5.690 | 1.00 23.87 |
| ATOM | 7801 | CD | ARG | 1145 | | -38.881 | 4.565 | 1.00 26.94 |
| ATOM | 7802 | NE | ARG | 1145 | | -40.162 | 5.055 | 1.00 27.22 |
| ATOM | 7803 | CZ | ARG | 1145 | | -40.448 -39.544 | 5.207 | 1.00 26.31 1.00 25.59 |
| ATOM | 7804 | NH1 | | 1145 | | -39.544 -41.646 | 4.909 5.639 | 1.00 25.59 1.00 27.26 |
| ATOM | 7805 | NH2 | AKG | 1145 | -0.407 | 41.040 | 5.037 | 1.00 2/.20 |

| ATOM 7806 C ARG 1145 -13.965 -37.865 8.050 1.00 22.32 ATOM 7808 N GLN 1146 -13.941 -38.685 9.098 1.00 21.32 ATOM 7809 CA GLN 1146 -13.941 -38.685 9.098 1.00 21.32 ATOM 7810 CB GLN 1146 -15.771 -39.190 9.701 1.00 22.47 ATOM 7811 CG GLN 1146 -16.081 -41.095 11.16 1.00 24.27 ATOM 7813 CEI GLN 1146 -15.732 -42.213 12.132 1.00 34.61 ATOM 7813 CEI GLN 1146 -15.732 -42.213 12.132 1.00 34.61 ATOM 7813 CEI GLN 1146 -16.081 -41.895 1.16 1.00 34.61 ATOM 7815 C GLN 1146 -15.732 -42.213 12.132 1.00 34.61 ATOM 7816 O GLN 1146 -16.382 -42.216 13.293 1.00 35.93 ATOM 7817 N TYR 1147 -15.918 -38.077 1.0423 1.00 22.67 ATOM 7818 CA TYR 1147 -15.774 -36.051 11.739 1.00 2.67 ATOM 7819 CB TYR 1147 -15.167 -37.165 11.027 1.00 22.67 ATOM 7820 CG TYR 1147 -15.167 -37.165 11.027 1.00 22.67 ATOM 7821 CD1 TYR 1147 -15.136 -33.900 12.979 1.00 21.86 ATOM 7822 CD1 TYR 1147 -16.312 -33.755 13.721 1.00 22.67 ATOM 7822 CD1 TYR 1147 -16.312 -33.755 13.721 1.00 22.56 ATOM 7824 CE2 TYR 1147 -16.312 -33.755 13.721 1.00 22.56 ATOM 7825 CZ TYR 1147 -16.312 -33.755 13.721 1.00 22.56 ATOM 7825 CZ TYR 1147 -16.312 -33.755 13.721 1.00 22.56 ATOM 7825 CZ TYR 1147 -16.312 -33.755 13.721 1.00 22.56 ATOM 7825 CZ TYR 1147 -16.312 -33.755 13.721 1.00 22.56 ATOM 7825 CZ TYR 1147 -16.312 -33.755 13.721 1.00 22.56 ATOM 7825 CZ TYR 1147 -16.312 -33.755 13.721 1.00 22.56 ATOM 7825 CZ TYR 1147 -16.325 -33.300 12.979 1.00 22.56 ATOM 7825 CZ TYR 1147 -16.325 -33.300 12.979 1.00 22.56 ATOM 7825 CZ TYR 1147 -16.325 -33.300 13.90 1.00 22.97 ATOM 7825 CZ TYR 1147 -16.325 -33.300 13.90 1.00 22.97 ATOM 7826 C H TYR 1147 -16.325 -33.300 13.90 1.00 22.97 ATOM 7827 C TYR 1147 -16.325 -33.300 13.90 1.00 22.97 ATOM 7828 C H TYR 1147 -16.325 -33.300 13.90 1.00 22.97 ATOM 7828 C H TYR 1147 -16.325 -33.300 13.90 1.00 22.97 ATOM 7827 C TYR 1147 -16.325 -33.300 1.00 23.00 | | | | | | | | | |
|--|------|------|-----|-----|------|---------|---------|--------|------------|
| Arrom 7808 N GLN 1146 -13.941 -38.685 9.098 1.00 21.32 Arrom 7807 CA GLN 1146 -15.771 -39.190 9.701 1.00 22.37 Arrom 7811 CB GLN 1146 -14.855 -40.318 10.691 1.00 24.27 Arrom 7811 CB GLN 1146 -16.081 -41.095 11.10 1.00 24.27 Arrom 7811 CB GLN 1146 -15.732 -42.213 12.132 1.00 34.61 Arrom 7813 CEI GLN 1146 -15.732 -42.213 12.132 1.00 34.61 Arrom 7814 NEZ GLN 1146 -16.382 -42.216 13.293 1.00 35.93 Arrom 7815 C GLN 1146 -16.382 -42.216 13.293 1.00 35.93 Arrom 7816 D GLN 1146 -15.918 -38.077 10.423 1.00 22.67 Arrom 7818 CA TYR 1147 -15.198 -38.077 10.423 1.00 22.67 Arrom 7818 CA TYR 1147 -15.167 -37.165 11.027 1.00 20.67 Arrom 7818 CA TYR 1147 -15.167 -37.165 11.027 1.00 22.67 Arrom 7820 CG TYR 1147 -15.167 -37.165 11.027 1.00 22.67 Arrom 7821 CDI TYR 1147 -15.136 -33.900 12.979 1.00 21.86 Arrom 7822 CEI TYR 1147 -15.136 -33.900 12.979 1.00 21.86 Arrom 7822 CEI TYR 1147 -16.312 -33.756 13.751 1.00 22.56 Arrom 7822 CEI TYR 1147 -16.312 -33.756 13.751 1.00 22.56 Arrom 7822 CEI TYR 1147 -16.312 -33.756 13.751 1.00 22.56 Arrom 7822 CEI TYR 1147 -16.312 -33.756 13.751 1.00 22.56 Arrom 7824 CEZ TYR 1147 -16.748 -32.511 14.186 1.00 21.50 Arrom 7824 CEZ TYR 1147 -16.745 -30.152 14.358 1.00 21.72 Arrom 7824 CEZ TYR 1147 -16.745 -30.152 14.358 1.00 21.72 Arrom 7826 CH TYR 1147 -16.599 -35.161 10.739 1.00 22.56 Arrom 7826 CH TYR 1147 -16.599 -35.161 10.739 1.00 22.56 Arrom 7826 CH TYR 1147 -16.599 -35.161 10.739 1.00 22.56 Arrom 7828 N MET 1148 -16.599 -35.161 10.739 1.00 22.47 Arrom 7831 CB MET 148 -14.484 -34.051 8.688 1.00 22.47 Arrom 7831 CB MET 148 -14.484 -34.051 8.688 1.00 22.47 Arrom 7831 CB MET 148 -14.484 -34.051 8.688 1.00 22.47 Arrom 7831 CB MET 148 -14.482 -30.152 14.358 1.00 23.56 Arrom 7831 CB MET 148 -14.192 -19.939 -31.330 6.619 1.00 23.56 Arrom 7837 N MLR 1149 -19.94 -36.868 1.00 22.47 Arrom 7837 N MLR 1149 -19.94 -36.868 1.00 22.47 Arrom 7837 N MLR 1149 -19.94 -36.868 1.00 22.47 Arrom 7837 N MLR 1149 -19.94 -36.868 1.00 22.40 1.00 23.60 Arrom 7845 CG GLU 1150 -20.27 -39.506 13.984 1.00 23.60 Arrom 7847 CG GLU | MOTA | 7806 | С | ARG | 1145 | -13.965 | -37.865 | 8.050 | 1.00 22.32 |
| ATOM 7809 CA GLN 1146 -15.171 -39.190 9.701 1.00 22.69 ATOM 7811 CB GLN 1146 -16.081 -41.095 11.161 1.00 29.43 ATOM 7812 CD GLN 1146 -16.081 -41.095 11.161 1.00 29.43 ATOM 7813 CEL GLN 1146 -16.081 -41.095 11.161 1.00 29.43 ATOM 7815 CC GLN 1146 -16.382 -42.213 12.13 1.00 34.63 ATOM 7815 C GLN 1146 -15.732 -42.213 12.13 1.00 34.63 ATOM 7815 C GLN 1146 -15.918 -38.077 10.423 1.00 25.56 ATOM 7816 O GLN 1146 -15.918 -38.077 10.423 1.00 22.56 ATOM 7817 N TYR 1147 -15.167 -37.165 11.027 1.00 20.38 ATOM 7818 CA TYR 1147 -15.167 -37.165 11.027 1.00 20.38 ATOM 7818 CA TYR 1147 -15.167 -37.165 11.027 1.00 20.38 ATOM 7819 CB TYR 1147 -16.312 -33.756 12.478 1.00 20.90 ATOM 7821 CDL TYR 1147 -16.312 -33.756 13.721 1.00 20.32 ATOM 7822 CEL TYR 1147 -16.312 -33.756 13.721 1.00 20.32 ATOM 7822 CEL TYR 1147 -16.312 -33.756 13.721 1.00 20.32 ATOM 7825 CZ TYR 1147 -16.315 -31.509 13.180 1.00 20.91 ATOM 7826 CD TYR 1147 -16.315 -31.509 13.180 1.00 20.91 ATOM 7827 C TYR 1147 -16.345 -30.152 14.388 1.00 21.00 ATOM 7828 O TYR 1147 -16.345 -30.152 14.388 1.00 21.01 ATOM 7828 O TYR 1147 -16.359 -31.389 13.910 1.00 22.56 ATOM 7829 N MET 1148 -16.345 -30.152 14.388 1.00 21.21 ATOM 7829 N MET 1148 -15.855 -34.881 9.618 1.00 22.47 ATOM 7829 N MET 1148 -15.855 -34.881 9.618 1.00 22.47 ATOM 7831 CB MET 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7838 CA MET 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7838 CA MET 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7838 CA MET 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7838 CA MET 1148 -15.427 -33.835 7.459 1.00 24.74 ATOM 7838 CA MET 1148 -15.427 -33.835 7.459 1.00 24.74 ATOM 7838 CA MET 1148 -15.427 -33.835 7.459 1.00 24.74 ATOM 7838 CA MET 1148 -15.427 -33.835 7.459 1.00 24.74 ATOM 7838 CA MET 1148 -15.427 -33.835 7.459 1.00 24.74 ATOM 7838 CA MET 1148 -15.427 -33.835 7.459 1.00 24.74 ATOM 7838 CA MET 1148 -15.427 -33.835 7.459 1.00 24.74 ATOM 7838 CA MET 1148 -15.427 -33.835 10.309 1.00 24.74 ATOM 7838 CA MET 1148 -15.427 -33.835 10.309 1.00 24.74 ATOM 7838 CA MET 1148 -15.427 -33.835 10.309 1.00 24 | MOTA | 7807 | 0 | ARG | 1145 | -15.010 | -37.470 | 7.531 | 1.00 22.86 |
| ATOM 7810 CB GIN 1146 -14.855 -40.318 10.691 1.00 24.27 ATOM 7812 CD GIN 1146 -15.732 -42.213 12.132 1.00 34.61 ATOM 7813 OEI GIN 1146 -15.732 -42.213 12.132 1.00 34.61 ATOM 7814 NEZ GIN 1146 -16.382 -42.216 13.293 1.00 35.93 ATOM 7816 C GIN 1146 -16.382 -42.216 13.293 1.00 35.93 ATOM 7816 C GIN 1146 -15.918 -38.077 10.423 1.00 22.67 ATOM 7817 N TYR 1147 -15.1918 -38.048 10.448 1.00 19.62 ATOM 7818 CA TYR 1147 -15.167 -37.165 11.079 1.00 22.67 ATOM 7819 CB TYR 1147 -15.167 -37.165 11.079 1.00 22.67 ATOM 7810 CB TYR 1147 -15.167 -37.165 11.079 1.00 22.67 ATOM 7820 CB TYR 1147 -15.167 -37.165 11.079 1.00 22.67 ATOM 7821 CD TYR 1147 -16.312 -33.756 13.729 1.00 22.67 ATOM 7822 CEI TYR 1147 -16.312 -33.756 13.751 1.00 21.86 ATOM 7823 CD TYR 1147 -16.312 -33.756 13.751 1.00 21.50 ATOM 7823 CD TYR 1147 -16.312 -33.756 13.751 1.00 22.67 ATOM 7825 CZ TYR 1147 -16.718 -32.511 14.186 1.00 21.50 ATOM 7826 CH TYR 1147 -16.312 -33.1389 13.90 1.00 22.57 ATOM 7827 C TYR 1147 -16.599 -31.389 13.90 1.00 22.57 ATOM 7827 C TYR 1147 -16.599 -31.389 13.90 1.00 22.57 ATOM 7828 O TYR 1147 -16.599 -31.389 13.90 1.00 22.57 ATOM 7829 N MET 1148 -15.855 -34.881 9.618 1.00 21.71 ATOM 7828 O TYR 1147 -16.599 -31.389 13.90 1.00 22.56 ATOM 7830 CA MET 1148 -16.599 -31.61 10.737 1.00 22.71 ATOM 7831 CB MET 1148 -16.484 3.47.52 10.969 1.00 23.56 ATOM 7832 CG MET 1148 -16.484 3.47.52 10.969 1.00 23.56 ATOM 7837 N ALA 1149 -15.457 -33.31 0.66 1.00 23.31 ATOM 7838 CA MET 1148 -15.427 -33.31 0.66 1.00 23.31 ATOM 7837 N ALA 1149 -17.764 3.34.752 10.00 29.93 ATOM 7838 CA LI 1149 -19.14 -36.828 8.079 1.00 24.94 ATOM 7836 C MET 1148 -17.791 -34.00 22.10 0.0 25.93 ATOM 7837 N ALA 1149 -19.14 -36.828 8.079 1.00 24.69 ATOM 7846 C G LU 1150 -20.228 37.742 1.00 22.00 2.00 2.00 2.00 2.00 2.00 2. | MOTA | 7808 | N | GLN | 1146 | -13.941 | -38.685 | 9.098 | 1.00 21.32 |
| ATOM 7811 CC GLN 1146 -16.081 -41.095 11.161 1.00 29.43 ATOM 7813 OEI GLN 1146 -15.732 -42.213 1.2132 1.00 36.88 ATOM 7815 C CLN 1146 -15.732 -42.216 13.293 1.00 35.93 ATOM 7815 C CLN 1146 -15.918 -38.048 1.04 1.02 22.57 ATOM 7816 O GLN 1146 -15.1574 -37.0555 11.027 1.00 20.38 ATOM 7819 CB TYR 1147 -15.774 -37.0555 11.027 1.00 20.20 22.67 ATOM 7821 CDI TYR 1147 -16.718 33.900 12.799 10.00 20.218 ATOM 7823 CDZ TYR 1147 -16.714 -14.769 -32.551 14.18 10.00 20.15 ATOM | MOTA | 7809 | CA | GLN | 1146 | -15.171 | -39.190 | 9.701 | 1.00 22.69 |
| ATOM Fall CD CLN 1146 -15.732 -42.213 21.312 1.00 34.61 ATOM Fall NEZ CLN 1146 -16.382 -42.216 13.293 1.00 36.88 ATOM Fall CD CLN 1146 -16.382 -42.216 13.293 1.00 36.88 ATOM Fall CD CLN 1146 -15.918 -38.077 10.423 1.00 22.56 ATOM Fall CD CLN 1146 -17.152 -38.048 10.448 1.00 19.62 ATOM Fall CD CLN 1147 -15.157 -37.165 11.027 1.00 20.38 ATOM Fall CD CLN 1147 -15.157 -36.051 11.739 1.00 22.57 ATOM Fall CD CLN 1147 -15.157 -36.051 11.739 1.00 20.90 ATOM Fall CD TWR 1147 -16.312 -33.756 13.721 1.00 20.32 ATOM Fall CD TWR 1147 -16.312 -33.756 13.721 1.00 20.32 ATOM Fall CD TWR 1147 -16.312 -33.756 13.721 1.00 20.32 ATOM Fall CD TWR 1147 -16.312 -33.756 13.121 1.00 20.56 ATOM Fall CD TWR 1147 -16.312 -33.756 13.121 1.00 20.56 ATOM Fall CD TWR 1147 -16.304 -33.556 13.121 1.00 20.56 ATOM Fall CD TWR 1147 -16.304 -33.556 13.180 1.00 20.76 ATOM Fall CD TWR 1147 -16.304 -33.556 13.180 1.00 20.76 ATOM Fall CD TWR 1147 -16.304 -33.556 13.180 1.00 20.75 ATOM Fall CD TWR 1147 -16.304 -33.556 13.891 1.00 22.56 ATOM Fall CD TWR 1147 -16.304 -33.556 13.891 1.00 22.56 ATOM Fall CD TWR 1147 -16.304 -33.556 13.891 1.00 22.56 ATOM Fall CD TWR 1147 -16.304 -33.556 13.891 0.00 22.56 ATOM Fall CD TWR 1147 -16.304 -33.556 13.891 0.00 22.56 ATOM Fall CD TWR 1148 -16.404 -34.0551 0.969 1.00 23.56 ATOM Fall CD TWR 1148 -16.404 -34.0551 0.969 1.00 23.56 ATOM Fall CD TWR 1148 -16.404 -34.0551 0.969 1.00 23.56 ATOM Fall CD TWR 1148 -16.404 -34.0551 0.969 1.00 23.66 ATOM Fall C | ATOM | 7810 | CB | GLN | 1146 | -14.855 | -40.318 | 10.691 | 1.00 24.27 |
| ATOM 7813 ORI GLN 1146 -14.892 -43.067 11.839 1.00 36.88 ATOM 7815 C GLN 1146 -15.918 -38.077 10.423 1.00 22.56 ATOM 7815 C GLN 1146 -15.918 -38.048 10.4293 1.00 22.56 ATOM 7816 O GLN 1146 -17.152 -38.048 10.428 1.00 22.56 ATOM 7817 N TYR 1147 -15.167 -37.165 11.027 1.00 20.38 ATOM 7818 CA TYR 1147 -15.774 -36.051 11.027 1.00 20.38 ATOM 7819 CB TYR 1147 -14.690 -35.256 12.478 1.00 20.90 20.67 ATOM 7820 CG TYR 1147 -14.690 -35.256 12.478 1.00 20.90 20.67 ATOM 7821 CDI TYR 1147 -16.312 -33.900 12.979 1.00 20.36 ATOM 7822 CEI TYR 1147 -16.312 -33.900 12.979 1.00 20.36 ATOM 7823 CDZ TYR 1147 -14.374 -32.511 14.86 1.00 20.35 ATOM 7823 CDZ TYR 1147 -14.374 -32.515 11.8186 1.00 20.76 ATOM 7825 CZ TYR 1147 -14.374 -32.515 11.8186 1.00 20.76 ATOM 7825 CZ TYR 1147 -16.365 30.152 14.358 1.00 20.76 ATOM 7825 CZ TYR 1147 -16.365 30.152 14.358 1.00 20.76 ATOM 7825 CZ TYR 1147 -16.365 30.152 14.358 1.00 21.72 ATOM 7828 O TYR 1147 -16.365 30.152 14.358 1.00 21.72 ATOM 7828 O TYR 1147 -16.365 34.7851 10.737 1.00 22.16 ATOM 7825 CZ TYR 1147 -16.509 -35.161 10.737 1.00 22.16 ATOM 7820 C MET 1148 -15.855 -34.881 9.618 1.00 22.47 ATOM 7830 C MET 1148 -15.474 -33.835 7.459 1.00 23.35 ATOM 7831 C MET 1148 -15.477 -33.835 7.459 1.00 23.31 ATOM 7831 C MET 1148 -15.477 -33.835 7.459 1.00 24.14 ATOM 7835 C MET 1148 -15.855 -34.881 9.618 1.00 22.474 ATOM 7835 C MET 1148 -15.855 -34.881 9.618 1.00 22.474 ATOM 7831 C MET 1148 -15.855 -34.881 9.618 1.00 22.474 ATOM 7835 C MET 1148 -15.855 -34.881 9.618 1.00 22.416 ATOM 7835 C MET 1148 -15.855 -34.881 9.618 1.00 22.416 ATOM 7835 C MET 1148 -15.855 -34.881 9.618 1.00 22.416 ATOM 7835 C MET 1148 -15.855 -34.881 9.618 1.00 22.416 ATOM 7835 C MET 1148 -15.855 -34.881 9.618 1.00 22.416 ATOM 7835 C MET 1148 -15.855 -34.881 9.618 1.00 22.416 ATOM 7835 C MET 1148 -15.855 -34.881 9.618 1.00 22.416 ATOM 7835 C MET 1148 -15.855 -34.881 9.618 1.00 22.416 ATOM 7835 C MET 1148 -15.855 -34.881 9.618 1.00 22.416 ATOM 7835 C MET 1148 -15.855 -34.881 9.618 1.00 22.575 ATOM 7835 C MET 1148 -15.855 -34.881 9.00 | MOTA | 7811 | CG | GLN | 1146 | -16.081 | | 11.161 | |
| ATOM 7814 NE2 GLM 1146 -16.382 -42.216 13.293 1.00 35.93 ATOM 7815 C GLM 1146 -17.152 -38.048 10.423 1.00 22.56 ATOM 7816 O GLM 1146 -17.152 -38.048 10.423 1.00 22.56 ATOM 7817 N TYR 1147 -15.167 -37.165 11.027 1.00 20.38 ATOM 7819 CB TYR 1147 -15.167 -37.165 11.027 1.00 20.39 ATOM 7819 CB TYR 1147 -15.167 -33.900 12.979 1.00 21.86 ATOM 7810 CB TYR 1147 -15.167 -33.900 12.979 1.00 21.86 ATOM 7821 CD1 TYR 1147 -16.312 -33.756 13.721 1.00 20.32 ATOM 7822 CEI TYR 1147 -16.312 -33.756 13.721 1.00 20.32 ATOM 7823 CD2 TYR 1147 -16.312 -33.756 13.721 1.00 20.32 ATOM 7823 CD2 TYR 1147 -16.312 -33.756 13.721 1.00 20.90 ATOM 7823 CD2 TYR 1147 -16.312 -33.756 13.180 1.00 20.76 ATOM 7826 CH TYR 1147 -16.325 11 14.186 1.00 21.50 ATOM 7826 CH TYR 1147 -16.599 -31.599 13.180 1.00 20.76 ATOM 7828 CH TYR 1147 -16.599 -31.599 13.180 1.00 20.76 ATOM 7828 CH TYR 1147 -16.599 -31.599 13.180 1.00 22.56 ATOM 7828 CH TYR 1147 -16.599 -31.590 13.180 1.00 22.56 ATOM 7828 CH TYR 1147 -16.599 -31.590 13.180 1.00 22.56 ATOM 7828 CH TYR 1147 -16.599 -35.152 10.737 1.00 22.11 ATOM 7828 CH TYR 1148 -15.855 -34.881 9.618 1.00 22.47 ATOM 7830 CA MET 1148 -15.427 -33.835 7.459 1.00 23.31 ATOM 7831 CA MET 1148 -15.427 -33.835 7.459 1.00 23.31 ATOM 7831 CH MET 1148 -15.427 -33.835 7.459 1.00 23.31 ATOM 7831 CH MET 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7835 CH MET 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7838 CH MET 1148 -15.437 -13.30 CH MET 1148 -12.910 -33.130 CH MET 1148 -12.910 CH MET 1148 -12.910 CH MET 1148 -12.910 CH MET 1148 -12.910 CH ME | MOTA | 7812 | CD | GLN | 1146 | -15.732 | | 12.132 | 1.00 34.61 |
| ATOM 7815 C GLN 1146 -15.918 -38.077 10.423 1.00 22.56 ATOM 7817 N TYR 1147 -15.167 -37.165 11.027 1.00 20.38 ATOM 7818 CA TYR 1147 -15.167 -37.165 11.027 1.00 20.38 ATOM 7819 CB TYR 1147 -15.774 -36.051 11.027 1.00 20.36 ATOM 7820 CG TYR 1147 -16.36.051 11.027 1.00 20.97 ATOM 7820 CG TYR 1147 -16.313 -33.900 12.979 1.00 21.86 ATOM 7821 CDI TYR 1147 -16.312 -33.900 12.979 1.00 21.86 ATOM 7822 CEI TYR 1147 -16.718 -32.511 14.186 1.00 21.50 ATOM 7823 CDZ TYR 1147 -16.718 -32.511 14.186 1.00 20.36 ATOM 7823 CDZ TYR 1147 -14.374 -32.579 12.719 1.00 20.91 ATOM 7825 CZ TYR 1147 -14.374 -32.579 12.719 1.00 20.91 ATOM 7825 CZ TYR 1147 -16.325 -33.500 12.729 1.00 20.76 ATOM 7825 CZ TYR 1147 -16.365 -30.152 14.358 1.00 21.72 ATOM 7828 O TYR 1147 -16.365 -30.152 14.358 1.00 21.72 ATOM 7828 O TYR 1147 -16.365 -34.881 9.518 1.00 22.56 ATOM 7820 CM BTY 1148 -15.855 -34.881 9.618 1.00 22.356 ATOM 7830 CA BTY 1148 -15.855 -34.881 9.618 1.00 23.356 ATOM 7831 CB BTY 1148 -15.427 -33.835 7.459 1.00 23.31 ATOM 7831 CB BTY 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7835 C BTY 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7835 C BTY 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7835 C BTY 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7835 C BTY 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7835 C BTY 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7835 C BTY 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7835 C BTY 1148 -15.865 -34.881 9.618 1.00 22.47 ATOM 7835 C BTY 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7835 C BTY 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7835 C BTY 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7835 C BTY 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7835 C BTY 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7835 C BTY 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7835 C BTY 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7835 C BTY 1148 -15.427 -33.835 7.459 1.00 24.14 ATOM 7835 C BTY 1148 -15.428 -348 -348 -348 -348 -348 -348 -348 -34 | MOTA | 7813 | | GLN | 1146 | | | | |
| ATOM 7816 O GLN 1146 -17.152 -38.048 10.448 1.00 19.62 0.38 ATOM 7817 N TYR 1147 -15.167 -37.165 11.027 1.00 20.38 ATOM 7818 CA TYR 1147 -15.167 -37.165 11.027 1.00 20.39 ATOM 7819 CB TYR 1147 -15.167 -35.256 12.478 1.00 20.90 ATOM 7820 CG TYR 1147 -15.136 -33.900 12.979 1.00 21.86 ATOM 7821 CD1 TYR 1147 -16.312 -33.756 13.721 1.00 20.32 ATOM 7823 CD2 TYR 1147 -16.312 -33.756 13.721 1.00 20.32 ATOM 7823 CD2 TYR 1147 -16.312 -33.756 13.721 1.00 20.31 ATOM 7823 CD2 TYR 1147 -16.312 -33.756 13.180 1.00 20.76 ATOM 7825 CZ TYR 1147 -14.376 -31.599 13.180 1.00 20.76 ATOM 7827 C TYR 1147 -16.599 -31.599 13.180 1.00 20.76 ATOM 7828 O TYR 1147 -16.509 -35.161 10.737 1.00 22.56 ATOM 7828 O TYR 1147 -16.509 -35.161 10.737 1.00 22.56 ATOM 7828 O TYR 1148 -15.855 -34.881 9.618 1.00 23.56 ATOM 7830 CA MET 1148 -15.855 -34.881 9.618 1.00 23.31 ATOM 7830 CA MET 1148 -15.427 -33.335 7.459 1.00 23.31 ATOM 7831 CC MET 1148 -15.427 -33.335 7.459 1.00 23.31 ATOM 7831 CC MET 1148 -15.427 -33.335 7.459 1.00 23.31 ATOM 7831 CC MET 1148 -15.427 -33.335 7.459 1.00 23.31 ATOM 7831 CC MET 1148 -15.427 -33.335 7.459 1.00 23.31 ATOM 7836 C MET 1148 -12.910 -33.130 6.619 1.00 23.93 ATOM 7835 C MET 1148 -12.910 -33.130 6.619 1.00 23.93 ATOM 7836 C MET 1148 -12.910 -33.130 6.619 1.00 22.95 ATOM 7837 C MET 1148 -12.910 -33.130 6.619 1.00 22.95 ATOM 7837 C MET 1148 -12.910 -33.130 6.619 1.00 22.95 ATOM 7837 C MET 1148 -17.701 -34.704 8.012 1.00 25.12 ATOM 7837 C MET 1148 -17.701 -34.704 8.012 1.00 25.12 ATOM 7837 C MET 1148 -17.701 -34.704 8.012 1.00 25.12 ATOM 7830 C MET 1148 -17.701 -34.704 8.012 1.00 25.12 ATOM 7830 C MET 1148 -17.701 -34.704 8.012 1.00 25.13 ATOM 7830 C MET 1148 -17.701 -34.704 8.012 1.00 25.12 ATOM 7830 C MET 1148 -17.701 -34.704 8.012 1.00 25.12 ATOM 7830 C MET 1148 -17.701 -34.704 8.012 1.00 25.12 ATOM 7830 C MET 1148 -17.701 -34.704 8.012 1.00 25.12 ATOM 7830 C MET 1148 -17.701 -34.704 8.012 1.00 25.26 ATOM 7830 C MET 1148 -17.701 -34.704 8.012 1.00 25.26 ATOM 7830 C MET 1148 -17.701 -34.704 8.012 1.00 25.26 ATOM 7830 C | MOTA | 7814 | NE2 | GLN | 1146 | | | | |
| ATOM 7817 N TYR 1147 -15.167 -37.165 11.027 1.00 20.38 ATOM 7818 C A TYR 1147 -14.690 -35.256 12.478 1.00 22.67 ATOM 7820 CG TYR 1147 -14.690 -35.256 12.478 1.00 20.90 21.86 ATOM 7821 CDI TYR 1147 -16.312 -33.790 12.799 1.00 21.86 ATOM 7823 CDZ TYR 1147 -16.312 -33.796 13.721 1.00 20.91 ATOM 7823 CDZ TYR 1147 -16.718 -32.511 14.86 1.00 20.91 ATOM 7825 CZ TYR 1147 -14.769 -31.599 13.180 1.00 20.91 ATOM 7825 CZ TYR 1147 -14.769 -31.599 13.180 1.00 20.91 ATOM 7825 CZ TYR 1147 -14.3769 -31.599 13.180 1.00 20.91 ATOM 7825 CZ TYR 1147 -16.599 -31.889 13.910 1.00 20.75 ATOM 7827 C TYR 1147 -16.599 -31.889 13.910 1.00 22.56 ATOM 7829 N TYR 1147 -16.599 -31.890 13.910 1.00 22.56 ATOM 7829 N TYR 1148 -15.855 -34.881 9.618 1.00 22.47 ATOM 7831 CB MET 1148 -15.855 -34.881 9.618 1.00 22.47 ATOM 7831 CB MET 1148 -15.427 -33.355 T.459 1.00 22.41 ATOM 7831 CB MET 1148 -15.427 -33.355 T.459 1.00 22.356 ATOM 7831 CB MET 1148 -15.427 -33.355 T.459 1.00 22.41 ATOM 7835 C MET 1148 -12.910 -33.3130 6.619 1.00 22.97 ATOM 7835 C MET 1148 -12.910 -33.3130 6.619 1.00 22.897 ATOM 7835 C MET 1148 -12.910 -33.3130 6.619 1.00 22.897 ATOM 7836 O MET 1148 -17.701 -36.704 CM 7836 C MET 1148 -17.701 -36.704 CM 7836 C MET 1148 -18.704 -34.014 S M.201 1.00 24.14 ATOM 7836 C MET 1148 -18.704 -18.718 -36.747 7.133 1.00 24.17 ATOM 7836 C MET 1148 -18.704 -18.718 -36.747 7.133 1.00 24.17 ATOM 7836 C MET 1148 -18.704 -18.718 -36.747 7.7133 1.00 24.17 ATOM 7836 C MET 1148 -18.704 -18.718 -36.747 7.7133 1.00 24.17 ATOM 7836 C MET 1148 -18.704 -18.718 -36.747 7.7133 1.00 24.18 ATOM 7836 C MET 1148 -18.704 -18.718 -36.747 7.7133 1.00 24.28 ATOM 7836 C MET 1148 -18.704 -18.718 -36.747 7.7133 1.00 24.28 ATOM 7836 C MET 1148 -18.704 -18.718 -1 | MOTA | | | | | | | | |
| ATOM 7818 CA TYR 1147 -14.690 -35.256 12.478 1.00 22.67 ATOM 7820 CG TYR 1147 -15.136 -33.900 12.979 1.00 20.93 ATOM 7821 CEI TYR 1147 -16.312 -33.756 13.721 1.00 20.150 ATOM 7824 CEZ TYR 1147 -16.312 -33.599 13.910 1.00 20.150 ATOM 7824 CEZ TYR 1147 -16.345 -30.152 11.00 20.150 ATOM 7827 C TYR 1147 -16.679 -31.599 13.180 1.00 22.56 ATOM 7837 C TYR 1147 -16.6599 -35.161 10.737 1.00 22.15 ATOM 7831 CB MET 1148 -15.855 -34.881 9.618 1.00 22.1 ATOM 7833 CB MET <t< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></t<> | | | | | | | | | |
| ATOM 7819 CB TYR 1147 -14.690 -35.256 12.478 1.00 20.90 ATOM 7821 CDI TYR 1147 -16.312 -33.756 13.721 1.00 21.03 ATOM 7823 CDE TYR 1147 -16.718 -32.511 14.186 1.00 20.32 ATOM 7823 CDE TYR 1147 -14.374 -32.511 14.186 1.00 20.91 ATOM 7825 CZ TYR 1147 -15.939 -31.389 13.910 1.00 20.76 ATOM 7826 O TYR 1147 -16.509 -35.161 10.737 1.00 22.15 ATOM 7830 C TYR 1147 -16.345 -30.152 10.959 1.00 22.56 ATOM 7831 CB MET 1148 -15.247 -33.130 1.00 22.56 ATOM 7834 CE MET 1 | | | | | | | | | |
| ATOM 7820 CC TYR 1147 -16.312 -33.756 13.721 1.00 20.36 ATOM 7822 CEI TYR 1147 -16.312 -33.756 13.721 1.00 20.35 ATOM 7823 CEZ TYR 1147 -14.374 -32.5151 14.166 1.00 20.150 ATOM 7824 CEZ TYR 1147 -14.7769 -31.509 13.180 1.00 20.76 ATOM 7825 OF TYR 1147 -16.345 -30.152 14.388 1.00 22.15 ATOM 7827 OF TYR 1147 -16.509 -35.161 10.737 1.00 22.15 ATOM 7831 CB MET 1148 -15.855 -34.881 9.618 1.00 22.17 ATOM 7831 CB MET 1148 -15.427 -33.305 7.679 1.00 25.93 ATOM 7833 CB | | | | | | | | | |
| ATOM 7821 CDI TYR 1147 -16.312 -33.756 13.721 1.00 20.32 ATOM 7822 CDI TYR 1147 -16.718 -32.511 14.186 1.00 21.00 20.91 ATOM 7825 CZ TYR 1147 -14.769 -31.509 13.180 1.00 20.91 ATOM 7825 CZ TYR 1147 -16.509 -31.589 13.180 1.00 22.56 ATOM 7826 O TYR 1147 -16.509 -35.161 10.737 1.00 22.172 ATOM 7830 CA MET 1148 -16.641 -34.051 8.580 1.00 22.55 ATOM 7831 CB MET 1148 -15.427 -33.835 7.459 1.00 24.93 ATOM 7832 CB MET 1148 -12.927 -33.350 7.869 1.00 24.93 ATOM 7834 < | | | | | | | | | |
| ATOM 7822 CEI TWR 1147 | | | | | | | | | |
| ATOM 7823 CD2 TYR 1147 -14.769 -31.509 13.180 1.00 20.91 ATOM 7825 CZ TYR 1147 -14.769 -31.509 -31.389 13.910 1.00 22.56 ATOM 7827 C TYR 1147 -16.599 -31.389 13.910 1.00 22.56 ATOM 7827 C TYR 1147 -16.599 -31.61 10.737 1.00 22.55 ATOM 7830 C MET 1148 -16.441 -34.051 8.580 1.00 22.59 ATOM 7831 CB MET 1148 -16.441 -33.307 7.879 1.00 25.93 ATOM 7834 CE MET 1148 -12.910 -33.130 6.619 1.00 28.79 ATOM 7834 CE MET 1148 -12.929 -33.920 7.00 6.10 22.93 ATOM 7835 CE | | | | | | | | | |
| ATOM 7824 CE2 TYR 1147 -14.769 -31.509 13.180 1.00 20.76 ATOM 7825 CZ TYR 1147 -16.345 -30.152 14.358 1.00 21.72 ATOM 7828 O TYR 1147 -16.509 -35.161 10.737 1.00 22.17 ATOM 7829 N MET 1148 -16.444 -34.051 8.580 1.00 22.37 ATOM 7831 CB MET 1148 -16.1855 -34.881 96.18 1.00 22.47 ATOM 7831 CB MET 1148 -16.5427 -33.835 7.459 1.00 25.93 ATOM 7833 SD MET 1148 -12.910 -33.130 6.619 1.00 28.97 ATOM 7835 C MET 1148 -117.701 -34.704 8.810 1.00 24.14 ATOM 7836 O MET< | | | | | | | | | |
| ATOM 7825 CZ TYR 1147 -15.939 -31.389 13.910 1.00 22.56 ATOM 7826 OH TYR 1147 -16.509 -35.161 10.737 1.00 22.15 ATOM 7829 N MET 1148 -15.855 -34.881 9.618 1.00 22.56 ATOM 7830 CA MET 1148 -15.427 -33.835 7.459 1.00 23.31 ATOM 7831 CB MET 1148 -15.441 -33.3075 7.879 1.00 25.93 ATOM 7834 CE MET 1148 -12.910 -33.130 6.619 1.00 28.93 ATOM 7835 CE MET 1148 -12.910 -33.130 6.619 1.00 28.93 ATOM 7834 CE MET 1148 -12.959 -3.700 1.00 28.193 ATOM 7835 CA MET 1148 <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> | | | | | | | | | |
| ATOM 78.26 OH TYR 1147 -16.345 -30.152 14.358 1.00 21.72 ATOM 78.27 C TYR 1147 -16.699 -35.161 10.737 1.00 22.17 ATOM 78.30 CA ETYR 1147 -17.643 -34.881 9.618 1.00 23.56 ATOM 78.31 CB MET 1148 -16.441 -34.051 8.580 1.00 22.37 ATOM 78.33 D MET 1148 -16.441 -34.055 7.879 1.00 25.97 ATOM 78.33 D MET 1148 -12.910 -33.130 6.619 1.00 28.97 ATOM 78.35 C MET 1148 -13.794 8.012 1.00 25.12 ATOM 78.35 C MET 1148 -13.797 -34.704 8.012 1.00 24.49 ATOM 78.36 C MET 1148< | | | | | | | | | |
| ATOM 7828 C TYR 1147 -16.509 -35.161 10.737 1.00 22.11 ATOM 7828 N MET 1148 -15.855 -34.881 9.618 1.00 22.47 ATOM 7830 Ca MET 1148 -15.855 -34.881 9.618 1.00 22.47 ATOM 7831 CB MET 1148 -15.855 -34.881 9.618 1.00 22.97 ATOM 7832 CC MET 1148 -15.872 -33.3075 7.879 1.00 25.93 ATOM 7834 CE MET 1148 -12.910 -33.130 6.619 1.00 28.93 ATOM 7835 C MET 1148 -17.770 -34.035 7.868 1.00 24.18 ATOM 7836 C MET 1148 -17.599 -35.992 7.700 1.00 24.28 ATOM/*7840 C ALA | | | | | | | | | |
| ATOM 7828 O TYR 1147 | | | | | | | | | |
| ATOM 7829 N MET 1148 | | | | | | | | | |
| ATOM | | | | | | | | | |
| ATOM 7831 CB MET 1148 | | | | | | | | | |
| ATOM 7832 CC MET 1148 | | | | | | | | | |
| ATOM 7833 SD MET 148 | | | | | | | | | |
| ATOM 7834 CE MET 1148 -13.585 -32.034 5.386 1.00 28.81 ATOM 7835 C MET 1148 -17.701 -34.704 8.012 1.00 25.12 ATOM 7836 O MET 1148 -18.743 -34.055 7.868 1.00 24.49 ATOM 7837 N ALA 1149 -17.599 -35.992 7.700 1.00 24.17 ATOM 7838 CA ALA 1149 -17.599 -35.992 7.700 1.00 24.12 ATOM 7839 CB ALA 1149 -18.718 -36.6747 7.133 1.00 24.28 ATOM 7840 C ALA 1149 -18.254 -38.152 6.750 1.00 23.46 ATOM 7841 O ALA 1149 -21.058 -36.613 7.669 1.00 23.46 ATOM 7842 N GLU 1150 -20.739 -37.135 9.346 1.00 24.16 ATOM 7843 CA GLU 1150 -20.739 -37.235 10.319 1.00 26.28 ATOM 7844 CB GLU 1150 -20.739 -37.235 10.319 1.00 26.28 ATOM 7845 CG GLU 1150 -20.156 -39.347 11.608 1.00 27.57 ATOM 7846 CD GLU 1150 -20.027 -39.506 13.984 1.00 28.17 ATOM 7847 OE1 GLU 1150 -20.027 -39.506 13.984 1.00 28.17 ATOM 7848 CD GLU 1150 -20.027 -39.506 13.984 1.00 28.17 ATOM 7850 C GLU 1150 -20.027 -39.506 13.984 1.00 28.42 ATOM 7851 N VAL 1151 -20.685 -34.888 10.408 1.00 27.27 ATOM 7852 CA VAL 1151 -20.685 -34.888 10.408 10.00 27.27 ATOM 7853 CB VAL 1151 -20.685 -34.888 10.408 10.00 27.27 ATOM 7853 CB VAL 1151 -20.685 -34.888 10.408 10.00 27.27 ATOM 7854 CG GLU 1150 -20.179 -32.384 10.668 10.00 27.12 ATOM 7856 C VAL 1151 -20.835 -31.005 10.609 1.00 23.63 ATOM 7857 C GLU 1152 -22.242 -33.154 9.495 1.00 28.77 ATOM 7858 N GLU 1152 -22.242 -33.154 9.495 1.00 28.77 ATOM 7858 N GLU 1152 -22.242 -33.154 9.495 1.00 28.77 ATOM 7858 N GLU 1152 -22.242 -33.154 9.495 1.00 38.92 ATOM 7860 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7860 CB GLU 1152 -22.641 -32.777 9.749 1.00 28.77 ATOM 7867 N SER 1153 -22.242 -33.154 9.495 1.00 38.93 ATOM 7867 N SER 1153 -22.242 -33.154 9.495 1.00 38.93 ATOM 7860 CB GLU 1152 -22.641 -32.777 9.749 1.00 33.92 ATOM 7867 N SER 1153 -22.242 -33.154 9.495 1.00 33.92 ATOM 7867 N SER 1153 -22.484 -37.534 7.468 1.00 34.62 ATOM 7867 N SER 1153 -22.484 -37.534 7.468 1.00 34.62 ATOM 7867 N SER 1153 -22.494 -33.456 6.60 1.00 35.70 ATOM 7867 N SER 1153 -22.494 -33.456 6.00 1.00 35.70 ATOM 7878 C GLU 1155 -22.597 -35.890 1.190 3.985 ATOM 7878 C GLU 1152 | | | | | | | | | |
| ATOM 7835 C MET 1148 -17.701 -34.704 8.012 1.00 25.12 ATOM 7836 O MET 1148 -18.743 -34.055 7.868 1.00 24.49 ATOM 7837 N ALA 1149 -17.599 -35.992 7.700 1.00 24.17 ATOM 7838 CA ALA 1149 -18.718 -36.747 7.133 1.00 24.28 ATOM 7839 CB ALA 1149 -18.254 -38.152 6.750 1.00 23.46 ATOM 7841 O ALA 1149 -19.914 -36.828 8.079 1.00 23.46 ATOM 7841 O ALA 1149 -19.914 -36.828 8.079 1.00 24.06 ATOM 7842 N GLU 1150 -19.657 -37.135 9.346 1.00 24.16 ATOM 7843 CA GLU 1150 -20.739 -37.235 10.319 1.00 24.26 ATOM 7844 CB GLU 1150 -20.739 -37.235 10.319 1.00 26.28 ATOM 7845 CG GLU 1150 -20.156 -39.347 11.608 1.00 28.54 ATOM 7846 CD GLU 1150 -19.614 -39.939 12.890 1.00 28.54 ATOM 7847 CEI GLU 1150 -20.027 -39.506 13.984 1.00 28.42 ATOM 7848 OE2 GLU 1150 -20.156 -39.347 11.608 1.00 28.54 ATOM 7850 C GLU 1150 -22.597 -35.859 10.949 1.00 28.42 ATOM 7851 N VAL 1151 -20.685 -34.808 10.408 1.00 27.27 ATOM 7852 CA VAL 1151 -20.685 -34.808 10.408 1.00 27.27 ATOM 7853 CB VAL 1151 -20.685 -34.808 10.408 1.00 27.27 ATOM 7854 CG1 VAL 1151 -20.685 -34.808 10.408 1.00 27.27 ATOM 7855 CG2 VAL 1151 -20.179 -32.384 10.668 1.00 27.12 ATOM 7856 C VAL 1151 -20.179 -32.384 10.668 1.00 27.12 ATOM 7857 C VAL 1151 -20.179 -32.384 10.669 1.00 23.64 ATOM 7858 N GLU 1152 -22.1792 -33.304 8.256 1.00 33.63 ATOM 7856 C VAL 1151 -22.242 -33.154 9.495 1.00 28.77 ATOM 7857 C C VAL 1151 -22.242 -33.3146 9.495 1.00 28.71 ATOM 7856 C VAL 1151 -22.384 -32.777 9.799 1.00 28.77 ATOM 7857 C C GLU 1152 -22.647 -32.998 7.112 1.00 33.63 ATOM 7858 N GLU 1152 -22.647 -32.998 7.112 1.00 33.63 ATOM 7856 C S C WAL 1151 -22.384 -32.777 9.49 1.00 23.64 ATOM 7856 C S C WAL 1151 -22.384 -32.777 9.49 1.00 23.64 ATOM 7856 C S C WAL 1152 -22.647 -32.998 7.112 1.00 33.93 ATOM 7860 C S GLU 1152 -22.647 -32.998 7.112 1.00 33.93 ATOM 7860 C S GLU 1152 -22.647 -32.998 7.112 1.00 33.93 ATOM 7860 C S C WAL 1151 -22.386 -33.496 6.640 1.00 34.62 ATOM 7867 N SER 1153 -24.942 -33.465 6.640 1.00 34.62 ATOM 7867 N SER 1153 -24.944 -38.999 1.00 35.70 ATOM 7867 C S C WAL 1155 -22.494 -33.690 1.00 3.00 3.9 | | | | | | | | | |
| ATOM 7836 O MET 1148 -18.743 -34.055 7.868 1.00 24.49 ATOM 7837 N ALA 1149 -17.599 -35.992 7.700 1.00 24.17 ATOM 7838 CA ALA 1149 -18.718 -36.747 7.133 1.00 24.28 ATOM 7839 CB ALA 1149 -18.254 -38.152 6.750 1.00 23.40 ATOM 7840 C ALA 1149 -19.914 -36.828 8.079 1.00 23.40 ATOM 7841 O ALA 1149 -21.058 -36.613 7.669 1.00 23.40 ATOM 7842 N GLU 1150 -20.739 -37.235 10.319 1.00 24.16 ATOM 7843 CA GLU 1150 -20.739 -37.235 10.319 1.00 26.28 ATOM 7846 CD GLU 1150 -20.156 -39.347 11.608 1.00 25.57 ATOM 7847 CE GLU 1150 -20.156 -39.347 11.608 1.00 25.57 ATOM 7848 OE2 GLU 1150 -20.027 -39.506 13.994 1.00 28.54 ATOM 7849 C GLU 1150 -20.027 -39.506 13.994 1.00 28.42 ATOM 7849 C GLU 1150 -20.027 -39.506 13.994 1.00 28.42 ATOM 7849 C GLU 1150 -22.027 -39.506 13.994 1.00 28.42 ATOM 7849 C GLU 1150 -22.027 -39.506 13.994 1.00 28.42 ATOM 7850 O GLU 1150 -22.597 -35.859 10.949 1.00 27.27 ATOM 7851 N VAL 1151 -22.2597 -35.859 10.949 1.00 27.27 ATOM 7852 CA VAL 1151 -20.685 -34.808 10.608 1.00 27.27 ATOM 7855 CG VAL 1151 -20.835 -31.005 10.609 1.00 23.63 ATOM 7856 CC VAL 1151 -20.835 -31.005 10.609 1.00 23.63 ATOM 7857 O VAL 1151 -22.242 -33.304 8.256 1.00 23.63 ATOM 7858 N GLU 1152 -22.1792 -33.304 8.256 1.00 33.92 ATOM 7859 CA GLU 1152 -22.199 -33.304 8.256 1.00 34.91 ATOM 7850 CB GLU 1152 -22.199 -33.304 8.256 1.00 34.91 ATOM 7851 N VAL 1151 -22.242 -33.304 8.256 1.00 34.91 ATOM 7856 CB GLU 1152 -22.199 -33.304 8.256 1.00 34.91 ATOM 7857 C VAL 1151 -22.242 -33.304 8.256 1.00 34.91 ATOM 7858 N GLU 1152 -22.199 -33.304 8.256 1.00 34.91 ATOM 7858 CG GLU 1152 -22.199 -33.304 8.256 1.00 34.91 ATOM 7860 CB GLU 1152 -22.199 -33.304 8.256 1.00 34.91 ATOM 7861 CG GLU 1152 -22.199 -33.304 8.256 1.00 34.91 ATOM 7862 CD GLU 1152 -22.199 -33.304 8.256 1.00 34.91 ATOM 7863 CE GLU 1152 -22.199 -33.304 8.256 1.00 34.91 ATOM 7864 CB GLU 1152 -22.3867 -33.895 7.051 1.00 34.67 ATOM 7867 N SER 1153 -22.494 -33.502 9.692 1.00 34.67 ATOM 7867 N SER 1153 -22.494 -33.495 6.640 1.00 34.67 ATOM 7867 CB GLU 1152 -22.364 -37.926 6.650 1.00 34.67 ATOM 7867 C | | | | | | | | | |
| ATOM | | 7836 | 0 | MET | | -18.743 | -34.055 | 7.868 | 1.00 24.49 |
| ATOM 7849 CB ALA 1149 -18.254 -38.152 6.750 1.00 23.46 ATOM 7840 C ALA 1149 -19.914 -36.828 8.079 1.00 23.40 ATOM 7841 O ALA 1149 -19.914 -36.828 8.079 1.00 23.40 ATOM 7842 N GLU 1150 -20.1058 -36.613 7.669 1.00 23.40 ATOM 7843 CA GLU 1150 -20.739 -37.235 10.319 1.00 24.16 ATOM 7844 CB GLU 1150 -20.228 -37.828 11.634 1.00 27.57 ATOM 7845 CG GLU 1150 -20.126 -39.347 11.608 1.00 28.54 ATOM 7846 CD GLU 1150 -20.126 -39.347 11.608 1.00 28.54 ATOM 7847 OEI GLU 1150 -20.027 -39.506 13.984 1.00 28.17 ATOM 7848 OE2 GLU 1150 -20.027 -39.506 13.984 1.00 28.42 ATOM 7849 C GLU 1150 -21.421 -35.900 10.581 1.00 23.40 ATOM 7850 O GLU 1150 -21.421 -35.900 10.581 1.00 27.27 ATOM 7851 N VAL 1151 -20.685 -34.808 10.408 1.00 27.27 ATOM 7852 CA VAL 1151 -20.685 -34.808 10.606 1.00 27.27 ATOM 7855 CC VAL 1151 -20.179 -32.384 10.668 1.00 27.27 ATOM 7856 CC VAL 1151 -20.179 -32.384 10.668 1.00 27.12 ATOM 7857 O VAL 1151 -20.835 -31.005 10.609 1.00 23.63 ATOM 7858 N GLU 1152 -22.242 -33.154 9.495 1.00 28.77 ATOM 7858 N GLU 1152 -22.242 -33.314 9.495 1.00 28.77 ATOM 7858 N GLU 1152 -22.637 -32.998 7.112 1.00 28.71 ATOM 7860 CB GLU 1152 -22.779 -32.384 3.486 1.00 39.92 ATOM 7861 CG GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7862 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7863 OEI GLU 1152 -22.242 -33.314 9.495 1.00 28.77 ATOM 7866 O GLU 1152 -22.2637 -32.998 7.112 1.00 33.92 ATOM 7866 O GLU 1152 -22.386 -33.197 5.815 1.00 31.00 39.92 ATOM 7866 O GLU 1152 -22.2647 -32.774 4.567 1.00 38.13 ATOM 7866 O GLU 1152 -22.2647 -33.2512 1.945 1.00 34.76 ATOM 7867 N SER 1153 -24.844 -36.102 7.456 1.00 34.67 ATOM 7868 C GLU 1152 -22.2647 -33.354 6.640 1.00 35.70 ATOM 7866 O GLU 1152 -22.2647 -33.350 6.640 1.00 34.76 ATOM 7867 N SER 1153 -24.844 -36.102 7.456 1.00 34.67 ATOM 7876 C GLU 1152 -22.647 -33.350 6.640 1.00 35.70 ATOM 7877 N VAL 1155 -22.280 -35.302 9.692 1.00 32.97 ATOM 7878 C GLY 1154 -25.280 -35.302 9.692 1.00 32.97 ATOM 7877 N VAL 1155 -22.994 -38.208 12.558 1.00 32.97 ATOM 7878 C GLY 1154 -25.295 -36.090 11.912 1.00 27.31 AT | ATOM | 7837 | N | ALA | 1149 | -17.599 | -35.992 | 7.700 | 1.00 24.17 |
| ATOM 7840 C ALA 1149 -19.914 -36.828 8.079 1.00 24.06 ATOM 7841 N GLU 1150 -19.657 -37.135 9.346 1.00 24.16 ATOM 7842 N GLU 1150 -20.739 -37.235 10.319 1.00 24.16 ATOM 7843 CA GLU 1150 -20.739 -37.235 10.319 1.00 24.16 ATOM 7844 CB GLU 1150 -20.156 -39.347 11.634 1.00 27.57 ATOM 7845 CG GLU 1150 -20.156 -39.347 11.608 1.00 28.54 ATOM 7846 CD GLU 1150 -20.156 -39.347 11.608 1.00 28.54 ATOM 7847 OEI GLU 1150 -20.027 -39.506 13.984 1.00 28.42 ATOM 7848 OE2 GLU 1150 -20.027 -39.506 13.984 1.00 28.42 ATOM 7849 C GLU 1150 -20.027 -39.506 13.984 1.00 28.42 ATOM 7850 O GLU 1150 -21.421 -35.900 10.581 1.00 27.42 ATOM 7851 N VAL 1151 -22.685 -34.808 10.408 1.00 27.27 ATOM 7852 CA VAL 1151 -22.685 -34.808 10.408 1.00 27.27 ATOM 7853 CB VAL 1151 -22.685 -34.808 10.667 10.00 27.12 ATOM 7855 CG VAL 1151 -20.179 -32.384 10.668 1.00 27.12 ATOM 7856 C VAL 1151 -20.179 -32.384 10.668 1.00 27.12 ATOM 7857 N VAL 1151 -22.242 -33.154 9.495 1.00 28.71 ATOM 7858 N GLU 1152 -22.179 -33.304 8.256 1.00 28.71 ATOM 7858 N GLU 1152 -22.197 -33.304 8.256 1.00 28.71 ATOM 7860 CB GLU 1152 -22.197 -33.304 8.256 1.00 30.65 ATOM 7861 CG GLU 1152 -22.197 -33.304 8.256 1.00 30.65 ATOM 7863 CB GLU 1152 -22.197 -33.304 8.256 1.00 30.65 ATOM 7866 CB GLU 1152 -22.197 -33.304 8.256 1.00 30.65 ATOM 7867 N SER 1153 -22.242 -33.154 9.495 1.00 28.71 ATOM 7868 CB GLU 1152 -22.197 -33.304 8.256 1.00 30.65 ATOM 7860 CB GLU 1152 -22.197 -33.304 8.256 1.00 30.65 ATOM 7863 CB GLU 1152 -22.197 -33.304 8.256 1.00 30.65 ATOM 7864 CE2 GLU 1152 -22.197 -33.304 8.256 1.00 30.65 ATOM 7866 CB GLU 1152 -22.197 -33.304 8.256 1.00 30.65 ATOM 7867 N SER 1153 -24.244 -33.395 7.051 1.00 35.70 ATOM 7866 CB GLU 1152 -22.377 -32.545 3.345 1.00 31.00 30.65 ATOM 7867 N SER 1153 -22.484 -37.926 6.357 1.00 39.92 ATOM 7867 N SER 1153 -22.484 -37.926 6.357 1.00 39.92 ATOM 7868 CB SER 1153 -22.484 -37.926 6.357 1.00 39.98 ATOM 7870 C SER 1153 -22.494 -33.299 7.051 1.00 39.62 ATOM 7877 N VAL 1155 -22.994 -33.252 11.984 1.00 27.31 ATOM 7878 CA VAL 1155 -22.994 -33.252 11.984 1.00 27.31 A | ATOM | 7838 | CA | ALA | 1149 | -18.718 | -36.747 | 7.133 | 1.00 24.28 |
| ATOM 7841 O ALA 1149 -21.058 -36.613 7.669 1.00 23.40 ATOM 7842 N GLU 1150 -19.657 -37.135 9.346 1.00 24.16 ATOM 7843 CA GLU 1150 -20.739 -37.235 10.319 1.00 26.28 ATOM 7845 CG GLU 1150 -20.739 -37.235 10.319 1.00 27.57 ATOM 7845 CG GLU 1150 -20.166 -39.347 11.608 1.00 28.54 ATOM 7846 CD GLU 1150 -19.614 -39.939 12.890 1.00 28.17 ATOM 7847 OE1 GLU 1150 -19.614 -39.939 12.890 1.00 28.17 ATOM 7848 OE2 GLU 1150 -20.027 -39.506 13.984 1.00 28.42 ATOM 7848 OE2 GLU 1150 -20.027 -39.506 13.984 1.00 28.42 ATOM 7849 C GLU 1150 -21.421 -35.900 10.581 1.00 26.66 ATOM 7850 O GLU 1150 -22.597 -35.859 10.949 1.00 27.27 ATOM 7851 N VAL 1151 -20.685 -34.808 10.408 1.00 27.27 ATOM 7852 CA VAL 1151 -20.685 -34.808 10.408 1.00 27.27 ATOM 7853 CB VAL 1151 -20.685 -34.808 10.668 1.00 27.12 ATOM 7855 CG2 VAL 1151 -20.835 -31.005 10.609 1.00 23.63 ATOM 7856 C VAL 1151 -20.835 -31.005 10.609 1.00 23.64 ATOM 7856 C VAL 1151 -20.835 -31.005 10.609 1.00 23.64 ATOM 7857 O VAL 1151 -22.242 -33.154 9.495 1.00 28.77 ATOM 7858 N GLU 1152 -22.637 -32.512 11.945 1.00 28.77 ATOM 7859 CA GLU 1152 -22.637 -32.998 7.112 1.00 28.77 ATOM 7860 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7860 CB GLU 1152 -22.637 -32.545 3.345 1.00 34.31 ATOM 7863 CB GLU 1152 -22.8367 -33.174 9.495 1.00 28.77 ATOM 7863 CB GLU 1152 -22.8367 -33.174 9.495 1.00 28.77 ATOM 7863 CB GLU 1152 -22.8367 -33.185 1.00 34.31 ATOM 7866 C GLU 1152 -22.8367 -33.175 1.00 34.31 ATOM 7868 CA GER 1153 -22.242 -33.354 10.604 1.00 35.70 ATOM 7866 C GLU 1152 -22.377 -32.545 3.345 1.00 34.31 ATOM 7868 CA GER 1153 -22.484 -37.534 7.559 1.00 34.76 ATOM 7868 CA GER 1153 -22.484 -37.534 7.559 1.00 34.76 ATOM 7869 CB SER 1153 -22.494 -33.456 6.640 1.00 34.67 ATOM 7869 CB SER 1153 -22.494 -33.456 6.640 1.00 34.67 ATOM 7876 C GLU 1152 -22.3777 -35.545 3.345 1.00 34.76 ATOM 7877 N VAL 1155 -22.806 -35.302 9.692 1.00 34.76 ATOM 7877 N VAL 1155 -22.806 -35.302 9.692 1.00 34.76 ATOM 7878 CA GLY 1154 -25.952 -36.090 11.912 1.00 27.31 ATOM 7879 CB SER 1153 -22.494 -33.509 10.835 1.00 27.91 ATOM 7878 | MOTA | 7839 | CB | ALA | 1149 | -18.254 | -38.152 | 6.750 | 1.00 23.46 |
| ATOM 7842 N GLU 1150 -19.657 -37.135 9.346 1.00 24.16 ATOM 7843 CA GLU 1150 -20.739 -37.235 10.319 1.00 26.28 ATOM 7844 CB GLU 1150 -20.228 -37.828 11.634 1.00 27.57 ATOM 7845 CG GLU 1150 -20.156 -39.347 11.608 1.00 28.54 ATOM 7846 CD GLU 1150 -20.027 -39.506 13.984 1.00 28.17 ATOM 7847 OE1 GLU 1150 -20.027 -39.506 13.984 1.00 28.42 ATOM 7848 OE2 GLU 1150 -18.778 -40.857 12.796 1.00 33.92 ATOM 7850 O GLU 1150 -21.421 -35.900 10.581 1.00 26.66 ATOM 7851 N VAL 1151 -20.685 -34.808 10.408 1.00 27.42 ATOM 7852 CA VAL 1151 -20.685 -34.808 10.408 1.00 27.27 ATOM 7853 CB VAL 1151 -20.179 -32.384 10.668 1.00 27.12 ATOM 7855 CG2 VAL 1151 -20.835 -31.005 10.609 1.00 23.63 ATOM 7856 C VAL 1151 -22.242 -33.154 9.495 1.00 23.64 ATOM 7857 O VAL 1151 -22.2384 -32.777 9.749 1.00 28.77 ATOM 7858 N GLU 1152 -22.2331 4 9.495 1.00 28.71 ATOM 7850 CB GLU 1152 -22.637 -32.898 7.112 1.00 33.92 ATOM 7856 C VAL 1151 -22.243 -33.146 9.495 1.00 28.71 ATOM 7857 O VAL 1151 -22.242 -33.154 9.495 1.00 28.77 ATOM 7858 N GLU 1152 -22.243 -33.486 10.609 1.00 23.63 ATOM 7850 CB GLU 1152 -22.243 -33.146 9.495 1.00 28.77 ATOM 7850 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7860 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7860 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7861 CG GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7862 CD GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7864 OE2 GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7866 C G GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7866 C G GLU 1152 -22.377 4 4.567 1.00 38.13 ATOM 7867 N SER 1153 -23.709 -35.147 7.468 1.00 34.62 ATOM 7868 CA SER 1153 -23.645 -37.926 6.640 1.00 34.62 ATOM 7870 C SER 1153 -22.647 -33.895 7.051 1.00 34.76 ATOM 7867 N SER 1153 -23.645 -37.926 6.557 1.00 33.54 ATOM 7871 C SER 1153 -22.6494 -33.546 6.640 1.00 34.62 ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7874 CA SER 1153 -22.6494 -36.157 8.487 1.00 27.21 ATOM 7878 CA VAL 1155 -22.9494 -36.577 33.805 1.00 27.31 ATOM 7878 CA VAL 1155 -22.9494 -38.208 12.558 1.00 27.91 ATOM 7878 C | MOTA | 7840 | С | ALA | 1149 | -19.914 | -36.828 | | |
| ATOM 7844 CB GLU 1150 -20.739 -37.235 10.319 1.00 26.28 ATOM 7844 CB GLU 1150 -20.228 -37.828 11.634 1.00 27.57 ATOM 7845 CG GLU 1150 -20.156 -39.347 11.608 1.00 28.54 ATOM 7846 CD GLU 1150 -20.0156 -39.347 11.608 1.00 28.54 ATOM 7847 OE1 GLU 1150 -19.614 -39.939 12.890 1.00 28.17 ATOM 7847 OE1 GLU 1150 -20.027 -39.506 13.984 1.00 28.42 ATOM 7848 OE2 GLU 1150 -18.778 -40.857 12.796 1.00 33.92 ATOM 7850 O GLU 1150 -22.597 -35.859 10.949 1.00 26.66 ATOM 7851 N VAL 1151 -20.685 -34.808 10.408 1.00 27.27 ATOM 7851 N VAL 1151 -20.685 -34.808 10.408 1.00 27.27 ATOM 7853 CB VAL 1151 -20.179 -32.384 10.668 1.00 27.27 ATOM 7855 CG2 VAL 1151 -20.835 -31.005 10.609 1.00 23.63 ATOM 7855 CG2 VAL 1151 -20.835 -31.005 10.609 1.00 23.63 ATOM 7856 C VAL 1151 -22.242 -33.154 94.95 1.00 28.71 ATOM 7857 O VAL 1151 -22.242 -33.154 94.95 1.00 28.71 ATOM 7858 N GLU 1152 -22.637 -32.998 7.112 1.00 28.71 ATOM 7860 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7860 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7864 CG GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7864 CG GLU 1152 -22.836 -33.117 5.813 1.00 34.31 ATOM 7865 C GLU 1152 -22.836 -33.117 5.813 1.00 34.31 ATOM 7866 C GLU 1152 -22.836 -33.117 5.813 1.00 34.31 ATOM 7866 C GLU 1152 -22.836 -33.117 5.813 1.00 34.31 ATOM 7866 C GLU 1152 -22.836 -33.117 5.813 1.00 34.31 ATOM 7866 C GLU 1152 -22.8367 -32.401 2.240 1.00 33.92 ATOM 7866 C GLU 1152 -22.337 -32.401 2.240 1.00 33.92 ATOM 7866 C GLU 1152 -22.337 -32.401 2.240 1.00 34.70 ATOM 7867 N SER 1153 -22.4846 -37.534 7.559 1.00 34.76 ATOM 7868 CA SER 1153 -22.4846 -37.534 7.559 1.00 34.67 ATOM 7867 N SER 1153 -22.4846 -37.534 7.559 1.00 34.76 ATOM 7871 C SER 1153 -22.4846 -37.534 7.559 1.00 34.67 ATOM 7878 C GLY 1154 -25.280 -35.302 9.692 1.00 30.23 ATOM 7874 CA GLY 1154 -25.952 -36.090 11.912 1.00 27.91 ATOM 7875 C GLY 1154 -25.952 -36.090 11.912 1.00 27.91 ATOM 7877 N VAL 1155 -22.944 -38.208 12.558 1.00 27.91 ATOM 7878 CA VAL 1155 -22.944 -38.208 12.558 1.00 27.91 ATOM 7878 CA VAL 1155 -22.969 -39.252 11.984 1.00 27.92 A | MOTA | 7841 | 0 | ALA | 1149 | -21.058 | | 7.669 | 1.00 23.40 |
| ATOM 7844 CB GLU 1150 | ATOM | | N | GLU | 1150 | | | | |
| ATOM 7845 CG GLU 1150 | ATOM | | CA | GLU | | | | | |
| ATOM 7846 CD GLU 1150 -19.614 -39.939 12.890 1.00 28.17 ATOM 7847 OE1 GLU 1150 -20.027 -39.506 13.984 1.00 28.42 ATOM 7848 OE2 GLU 1150 -18.778 -40.857 12.796 1.00 23.42 ATOM 7849 C GLU 1150 -21.421 -35.900 10.581 1.00 26.66 ATOM 7850 O GLU 1150 -22.597 -35.859 10.949 1.00 27.42 ATOM 7851 N VAL 1151 -20.685 -34.808 10.408 1.00 27.27 ATOM 7852 CA VAL 1151 -20.685 -34.808 10.617 1.00 27.27 ATOM 7853 CB VAL 1151 -20.685 -34.808 10.668 1.00 27.27 ATOM 7854 CG1 VAL 1151 -20.835 -31.005 10.609 1.00 23.63 ATOM 7855 CG2 VAL 1151 -20.835 -31.005 10.609 1.00 23.63 ATOM 7856 CC VAL 1151 -22.242 -33.154 9.495 1.00 23.64 ATOM 7857 O VAL 1151 -22.242 -33.154 9.495 1.00 28.77 ATOM 7858 N GLU 1152 -22.2637 -32.998 7.112 1.00 30.65 ATOM 7850 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7860 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7861 CG GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7863 OE1 GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7866 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7866 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7866 OB GLU 1152 -22.641 -32.774 4.567 1.00 34.31 ATOM 7866 CB GLU 1152 -22.641 -32.774 4.567 1.00 34.31 ATOM 7866 CB GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7866 CB GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7866 CB GLU 1152 -22.3367 -33.895 7.051 1.00 34.76 ATOM 7866 CB GLU 1152 -22.3867 -33.895 7.051 1.00 34.76 ATOM 7867 N SER 1153 -24.844 -36.102 7.456 1.00 34.62 ATOM 7868 CA SER 1153 -24.844 -36.102 7.456 1.00 34.62 ATOM 7870 OG SER 1153 -24.844 -36.102 7.456 1.00 34.62 ATOM 7870 CG SER 1153 -22.645 -37.926 6.357 1.00 39.93 ATOM 7870 CG SER 1153 -22.645 -37.926 6.357 1.00 39.93 ATOM 7871 C SER 1153 -22.645 -37.926 6.357 1.00 39.86 ATOM 7873 N GLY 1154 -25.952 -36.090 11.912 1.00 27.31 ATOM 7878 CA VAL 1155 -22.969 -39.252 11.984 1.00 27.21 ATOM 7879 CB VAL 1155 -22.969 -39.252 11.984 1.00 27.21 ATOM 7878 CA VAL 1155 -22.4944 -38.208 12.558 1.00 27.31 ATOM 7878 CA VAL 1155 -22.4944 -38.208 12.558 1.00 27.31 ATOM 7878 CG VAL 1155 -22.4944 -38.208 12.558 1.0 | | | | | | | | | |
| ATOM 7847 OE1 GLU 1150 | | | | | | | | | |
| ATOM 7848 OE2 GLU 1150 | | | | | | | | | |
| ATOM 7849 C GLU 1150 -21.421 -35.900 10.581 1.00 26.66 ATOM 7850 O GLU 1150 -22.597 -35.859 10.949 1.00 27.27 ATOM 7851 N VAL 1151 -20.685 -34.808 10.408 1.00 27.27 ATOM 7852 CA VAL 1151 -20.685 -34.808 10.408 1.00 27.27 ATOM 7853 CB VAL 1151 -20.179 -32.384 10.668 1.00 27.27 ATOM 7854 CG1 VAL 1151 -20.179 -32.384 10.668 1.00 27.12 ATOM 7855 CG2 VAL 1151 -20.835 -31.005 10.609 1.00 23.63 ATOM 7855 CG2 VAL 1151 -29.835 -31.005 10.609 1.00 23.64 ATOM 7855 CG2 VAL 1151 -22.242 -33.154 9.495 1.00 28.77 ATOM 7857 O VAL 1151 -22.3384 -32.777 9.749 1.00 28.77 ATOM 7858 N GLU 1152 -22.637 -32.998 7.112 1.00 30.65 ATOM 7859 CA GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7860 CB GLU 1152 -22.637 -32.998 7.112 1.00 34.31 ATOM 7861 CG GLU 1152 -22.641 -32.774 4.567 1.00 34.31 ATOM 7862 CD GLU 1152 -22.337 -32.401 2.240 1.00 39.92 ATOM 7866 OE GLU 1152 -22.337 -32.401 2.240 1.00 39.92 ATOM 7866 OE GLU 1152 -22.337 -32.401 2.240 1.00 34.32 ATOM 7865 C GLU 1152 -22.337 -32.498 3.485 1.00 41.00 ATOM 7866 OE GLU 1152 -22.337 -32.498 3.485 1.00 41.00 ATOM 7866 OE GLU 1152 -22.337 -32.498 3.485 1.00 41.00 ATOM 7866 OE GLU 1152 -22.3867 -33.895 7.051 1.00 34.76 ATOM 7866 OE GLU 1152 -22.3867 -33.895 7.051 1.00 34.76 ATOM 7866 OE GLU 1152 -22.3867 -33.895 7.051 1.00 34.67 ATOM 7866 OE GLU 1152 -24.942 -33.456 6.640 1.00 35.70 ATOM 7866 OE GLU 1152 -24.842 -37.534 7.559 1.00 34.67 ATOM 7869 CB SER 1153 -24.814 -36.102 7.456 1.00 34.67 ATOM 7869 CB SER 1153 -24.814 -36.102 7.456 1.00 35.74 ATOM 7869 CB SER 1153 -24.814 -36.102 7.456 1.00 35.74 ATOM 7870 OG SER 1153 -24.814 -36.102 7.456 1.00 35.74 ATOM 7870 OG SER 1153 -24.814 -36.102 7.456 1.00 35.74 ATOM 7870 OG SER 1153 -24.814 -36.102 7.456 1.00 32.97 ATOM 7870 OG SER 1153 -24.814 -36.102 7.456 1.00 32.97 ATOM 7870 OG SER 1153 -24.814 -36.102 7.456 1.00 32.97 ATOM 7870 OG SER 1153 -24.814 -36.102 7.456 1.00 32.97 ATOM 7870 OG SER 1153 -24.846 -37.534 7.559 1.00 32.73 ATOM 7870 OG SER 1153 -24.846 -37.534 7.559 1.00 30.22 97 ATOM 7874 CA GLY 1154 -26.390 -39.525 1.00 30.02 2.97 | | | | | | | | | |
| ATOM 7850 O GLU 1150 -22.597 -35.859 10.949 1.00 27.42 ATOM 7851 N VAL 1151 -20.685 -34.808 10.408 1.00 27.27 ATOM 7852 CA VAL 1151 -20.685 -34.808 10.667 1.00 27.27 ATOM 7853 CB VAL 1151 -20.179 -32.384 10.668 1.00 27.12 ATOM 7854 CG1 VAL 1151 -20.835 -31.005 10.609 1.00 23.63 ATOM 7855 CG2 VAL 1151 -19.372 -32.512 11.945 1.00 23.64 ATOM 7856 C VAL 1151 -22.242 -33.154 9.495 1.00 28.77 ATOM 7857 O VAL 1151 -22.384 -32.777 9.749 1.00 28.77 ATOM 7858 N GLU 1152 -22.242 -33.304 8.256 1.00 30.65 ATOM 7859 CA GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7860 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7861 CG GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7862 CD GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7864 OE2 GLU 1152 -22.641 -32.774 4.567 1.00 39.92 ATOM 7866 C GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7866 C GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7866 C GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7866 C GLU 1152 -22.337 -32.401 2.240 1.00 34.76 ATOM 7867 N SER 1153 -24.984 -37.534 7.559 1.00 34.67 ATOM 7868 CA SER 1153 -24.284 -37.534 7.559 1.00 34.67 ATOM 7869 CB SER 1153 -24.284 -37.534 7.559 1.00 39.86 ATOM 7870 OG SER 1153 -24.284 -37.534 7.559 1.00 39.98 ATOM 7870 OG SER 1153 -24.284 -37.534 7.559 1.00 39.98 ATOM 7871 C SER 1153 -25.787 -35.850 9.692 1.00 30.02 ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 30.29 ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7874 CA GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7875 C GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7876 C GLY 1154 -25.280 -35.302 9.692 1.00 27.31 ATOM 7877 N VAL 1155 -22.197 -37.140 11.599 1.00 27.31 ATOM 7878 CA VAL 1155 -22.197 -37.140 11.599 1.00 27.31 ATOM 7879 CB VAL 1155 -23.969 -39.252 11.984 1.00 27.96 ATOM 7870 CG VAL 1155 -23.969 -39.252 11.984 1.00 27.92 ATOM 7880 CG1 VAL 1155 -23.969 -39.252 11.984 1.00 27.92 | | | | | | | | | |
| ATOM 7851 N VAL 1151 -20.685 -34.808 10.408 1.00 27.27 ATOM 7852 CA VAL 1151 -21.263 -33.486 10.617 1.00 27.27 ATOM 7853 CB VAL 1151 -20.179 -32.384 10.668 1.00 27.12 ATOM 7854 CG1 VAL 1151 -20.179 -32.384 10.668 1.00 27.12 ATOM 7855 CG2 VAL 1151 -20.179 -32.384 10.669 1.00 23.63 ATOM 7856 C VAL 1151 -19.372 -32.512 11.945 1.00 23.64 ATOM 7857 O VAL 1151 -22.242 -33.154 9.495 1.00 28.77 ATOM 7858 N GLU 1152 -21.792 -33.304 8.256 1.00 30.65 ATOM 7859 CA GLU 1152 -21.792 -33.304 8.256 1.00 30.65 ATOM 7860 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7861 CG GLU 1152 -22.637 -32.998 7.112 1.00 34.31 ATOM 7862 CD GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7863 OE1 GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7864 OE2 GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7865 C GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7866 O GLU 1152 -22.337 -32.498 3.485 1.00 34.76 ATOM 7866 O GLU 1152 -22.337 -32.498 3.485 1.00 34.76 ATOM 7866 O GLU 1152 -22.337 -32.498 3.485 1.00 34.76 ATOM 7866 O GLU 1152 -22.337 -32.401 2.240 1.00 33.70 ATOM 7867 N SER 1153 -23.764 -36.102 7.456 1.00 34.67 ATOM 7868 CA SER 1153 -24.814 -36.102 7.456 1.00 34.67 ATOM 7869 CB SER 1153 -24.814 -36.102 7.456 1.00 34.67 ATOM 7869 CB SER 1153 -24.814 -36.102 7.456 1.00 39.86 ATOM 7871 C SER 1153 -24.84 -37.534 7.559 1.00 35.72 ATOM 7872 O SER 1153 -24.84 -37.534 7.559 1.00 35.72 ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7874 CA GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7875 C GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7876 O GLY 1154 -26.130 -35.309 10.835 1.00 27.31 ATOM 7878 CA VAL 1155 -22.6494 -38.208 12.558 1.00 27.30 ATOM 7877 N VAL 1155 -22.728 -30.058 12.558 1.00 27.30 ATOM 7878 CA VAL 1155 -23.728 -30.252 11.984 1.00 27.31 ATOM 7879 CB VAL 1155 -23.728 -30.3828 10.692 1.00 30.23 ATOM 7880 CG1 VAL 1155 -23.728 -30.3582 10.692 1.00 30.23 | | | | | | | | | |
| ATOM 7852 CA VAL 1151 -21.263 -33.486 10.617 1.00 27.27 ATOM 7853 CB VAL 1151 -20.179 -32.384 10.668 1.00 27.12 ATOM 7854 CG1 VAL 1151 -20.835 -31.005 10.609 1.00 23.63 ATOM 7855 CG2 VAL 1151 -19.372 -32.512 11.945 1.00 23.64 ATOM 7856 C VAL 1151 -22.242 -33.154 9.495 1.00 28.77 ATOM 7857 O VAL 1151 -22.384 -32.777 9.749 1.00 28.71 ATOM 7858 N GLU 1152 -21.792 -33.304 8.256 1.00 30.65 ATOM 7859 CA GLU 1152 -21.792 -33.304 8.256 1.00 33.92 ATOM 7860 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7861 CG GLU 1152 -21.836 -33.117 5.813 1.00 34.31 ATOM 7862 CD GLU 1152 -21.836 -33.117 5.813 1.00 34.31 ATOM 7863 OEI GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7864 OE2 GLU 1152 -21.775 -32.545 3.345 1.00 39.92 ATOM 7865 C GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7866 O GLU 1152 -20.535 -32.498 3.485 1.00 41.00 ATOM 7866 O GLU 1152 -20.535 -32.498 3.485 1.00 41.00 ATOM 7866 O GLU 1152 -20.535 -32.498 3.485 1.00 34.76 ATOM 7868 CA SER 1153 -24.942 -33.456 6.640 1.00 35.70 ATOM 7868 CA SER 1153 -24.942 -33.456 6.640 1.00 35.70 ATOM 7868 CA SER 1153 -24.942 -33.456 6.640 1.00 35.72 ATOM 7869 CB SER 1153 -24.844 -37.534 7.559 1.00 39.86 ATOM 7870 OG SER 1153 -24.284 -37.534 7.559 1.00 39.86 ATOM 7871 C SER 1153 -22.6974 -36.157 8.487 1.00 39.86 ATOM 7872 O SER 1153 -22.5787 -35.852 8.596 1.00 32.97 ATOM 7873 N GLY 1154 -26.30 -35.302 9.692 1.00 30.02 ATOM 7874 CA GLY 1154 -26.130 -35.302 9.692 1.00 30.02 ATOM 7875 C GLY 1154 -26.130 -35.900 11.912 1.00 27.31 ATOM 7876 CA VAL 1155 -22.995 -36.090 11.912 1.00 27.31 ATOM 7877 N VAL 1155 -22.996 -39.252 11.984 1.00 27.92 ATOM 7879 CB VAL 1155 -22.969 -39.252 11.984 1.00 27.92 ATOM 7879 CB VAL 1155 -22.3969 -39.252 11.984 1.00 27.92 ATOM 7880 CG1 VAL 1155 -23.796 -39.828 10.692 1.00 30.23 | | | | | | | | | |
| ATOM 7853 CB VAL 1151 -20.179 -32.384 10.668 1.00 27.12 ATOM 7854 CG1 VAL 1151 -20.835 -31.005 10.609 1.00 23.63 ATOM 7855 CG2 VAL 1151 -19.372 -32.512 11.945 1.00 23.64 ATOM 7856 C VAL 1151 -22.242 -33.154 9.495 1.00 28.77 ATOM 7857 O VAL 1151 -22.384 -32.777 9.749 1.00 28.77 ATOM 7858 N GLU 1152 -21.792 -33.304 8.256 1.00 30.65 ATOM 7859 CA GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7860 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7861 CG GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7862 CD GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7863 OEI GLU 1152 -22.641 -32.774 4.567 1.00 39.92 ATOM 7864 OE2 GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7866 O GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7866 O GLU 1152 -22.337 -32.498 3.485 1.00 39.92 ATOM 7866 O GLU 1152 -22.3367 -33.895 7.051 1.00 34.76 ATOM 7866 C GLU 1152 -23.867 -33.895 7.051 1.00 34.76 ATOM 7866 C GEU 1152 -24.942 -33.456 6.640 1.00 35.70 ATOM 7868 CA SER 1153 -24.942 -33.456 6.640 1.00 35.70 ATOM 7869 CB SER 1153 -24.814 -36.102 7.456 1.00 34.62 ATOM 7870 OG SER 1153 -24.814 -36.102 7.456 1.00 34.62 ATOM 7871 C SER 1153 -22.6974 -35.852 8.596 1.00 32.97 ATOM 7872 O SER 1153 -22.6974 -36.157 8.487 1.00 32.97 ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 32.97 ATOM 7874 CA GLY 1154 -25.280 -35.302 9.692 1.00 32.97 ATOM 7875 C GLY 1154 -25.280 -35.302 9.692 1.00 27.31 ATOM 7876 O GLY 1154 -25.952 -36.090 11.912 1.00 27.31 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.31 ATOM 7878 CA VAL 1155 -22.4944 -38.208 12.558 1.00 27.32 ATOM 7879 CB VAL 1155 -22.3969 -39.252 11.984 1.00 27.32 ATOM 7880 CG1 VAL 1155 -22.3969 -39.252 11.984 1.00 27.32 | | | | | | | | | |
| ATOM 7854 CG1 VAL 1151 -20.835 -31.005 10.609 1.00 23.63 ATOM 7855 CG2 VAL 1151 -19.372 -32.512 11.945 1.00 23.64 ATOM 7856 C VAL 1151 -22.242 -33.154 9.495 1.00 28.77 ATOM 7857 O VAL 1151 -23.384 -32.777 9749 1.00 28.71 ATOM 7858 N GLU 1152 -21.792 -33.304 8.256 1.00 30.65 ATOM 7859 CA GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7860 CB GLU 1152 -21.836 -33.117 5.813 1.00 34.31 ATOM 7861 CG GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7862 CD GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7863 OE1 GLU 1152 -22.337 -32.498 3.485 1.00 43.20 ATOM 7864 OE2 GLU 1152 -22.337 -32.498 3.485 1.00 41.00 ATOM 7865 C GLU 1152 -22.535 -32.498 3.485 1.00 41.00 ATOM 7866 O GLU 1152 -23.867 -33.895 7.051 1.00 34.76 ATOM 7866 O GLU 1152 -24.942 -33.456 6.640 1.00 35.70 ATOM 7867 N SER 1153 -23.709 -35.147 7.468 1.00 34.67 ATOM 7869 CB SER 1153 -24.284 -37.534 7.559 1.00 34.67 ATOM 7869 CB SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7870 OG SER 1153 -24.284 -37.534 7.559 1.00 32.97 ATOM 7871 C SER 1153 -24.284 -37.534 7.559 1.00 32.97 ATOM 7872 O SER 1153 -23.645 -37.926 6.357 1.00 32.97 ATOM 7874 CA GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7875 C GLY 1154 -26.130 -35.302 10.835 1.00 27.96 ATOM 7876 O GLY 1154 -26.491 -35.960 13.008 1.00 27.96 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.21 ATOM 7878 CA VAL 1155 -22.728 -40.357 13.005 1.00 27.92 ATOM 7878 CA VAL 1155 -24.528 -39.828 10.692 1.00 30.23 ATOM 7878 CA VAL 1155 -23.728 -40.357 13.005 1.00 27.92 ATOM 7878 CA VAL 1155 -23.728 -40.357 13.005 1.00 27.92 ATOM 7878 CB VAL 1155 -23.728 -40.357 13.005 1.00 27.92 | | | | | | | | | |
| ATOM 7855 CG2 VAL 1151 -19.372 -32.512 11.945 1.00 23.64 ATOM 7856 C VAL 1151 -22.242 -33.154 9.495 1.00 28.77 ATOM 7857 O VAL 1151 -23.384 -32.777 9.749 1.00 28.77 ATOM 7858 N GLU 1152 -21.792 -33.304 8.256 1.00 30.65 ATOM 7859 CA GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7860 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7861 CG GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7862 CD GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7863 OE1 GLU 1152 -22.337 -32.945 3.345 1.00 39.92 ATOM 7864 OE2 GLU 1152 -22.337 -32.401 2.40 1.00 43.20 ATOM 7865 C GLU 1152 -22.337 -32.401 2.40 1.00 41.00 ATOM 7866 O GLU 1152 -22.3867 -33.895 7.051 1.00 34.76 ATOM 7866 O GLU 1152 -24.942 -33.456 6.640 1.00 35.70 ATOM 7867 N SER 1153 -23.709 -35.147 7.468 1.00 34.67 ATOM 7868 CA SER 1153 -24.844 -36.102 7.456 1.00 34.67 ATOM 7869 CB SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7870 OG SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7871 C SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7872 O SER 1153 -25.787 -35.852 8.596 1.00 32.97 ATOM 7874 CA GLY 1154 -25.280 -35.302 9.692 1.00 30.22 ATOM 7875 C GLY 1154 -26.130 -35.302 9.692 1.00 30.22 ATOM 7877 N VAL 1155 -25.280 -35.302 9.692 1.00 30.23 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.21 ATOM 7878 CA VAL 1155 -25.197 -37.140 11.599 1.00 27.21 ATOM 7878 CA VAL 1155 -23.728 -40.357 13.005 1.00 27.92 ATOM 7878 CA VAL 1155 -23.728 -40.357 13.005 1.00 27.92 ATOM 7878 CA VAL 1155 -23.728 -40.357 13.005 1.00 27.92 ATOM 7878 CA VAL 1155 -23.728 -40.357 13.005 1.00 27.92 | | | | | | | | | |
| ATOM 7856 C VAL 1151 -22.242 -33.154 9.495 1.00 28.77 ATOM 7857 O VAL 1151 -23.384 -32.777 9.749 1.00 28.71 ATOM 7858 N GLU 1152 -21.792 -33.304 8.256 1.00 30.65 ATOM 7859 CA GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7860 CB GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7861 CG GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7862 CD GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7863 OE1 GLU 1152 -21.775 -32.545 3.345 1.00 39.92 ATOM 7864 OE2 GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7865 C GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7866 O GLU 1152 -23.867 -33.895 7.051 1.00 34.76 ATOM 7866 O GLU 1152 -24.942 -33.456 6.640 1.00 35.70 ATOM 7867 N SER 1153 -23.709 -35.147 7.468 1.00 34.67 ATOM 7868 CA SER 1153 -24.284 -37.534 7.559 1.00 34.62 ATOM 7869 CB SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7870 OG SER 1153 -24.284 -37.534 7.559 1.00 39.86 ATOM 7871 C SER 1153 -23.645 -37.926 6.357 1.00 39.86 ATOM 7873 N GLY 1154 -25.280 -35.852 8.596 1.00 32.97 ATOM 7874 CA GLY 1154 -26.130 -35.039 10.835 1.00 27.31 ATOM 7876 O GLY 1154 -26.130 -35.039 10.835 1.00 28.64 ATOM 7877 N VAL 1155 -25.952 -36.090 11.912 1.00 27.31 ATOM 7878 CA VAL 1155 -22.4944 -38.208 12.558 1.00 27.92 ATOM 7879 CB VAL 1155 -22.4944 -38.208 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -22.4944 -38.208 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7879 CB VAL 1155 -23.728 -40.357 13.005 1.00 30.23 | | | | | | | | | |
| ATOM 7857 O VAL 1151 -23.384 -32.777 9.749 1.00 28.71 ATOM 7858 N GLU 1152 -21.792 -33.304 8.256 1.00 30.65 ATOM 7859 CA GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7860 CB GLU 1152 -21.836 -33.117 5.813 1.00 34.31 ATOM 7861 CG GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7862 CD GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7863 OE1 GLU 1152 -22.677 -32.545 3.345 1.00 39.92 ATOM 7864 OE2 GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7865 C GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7866 O GLU 1152 -22.337 -32.498 3.485 1.00 41.00 ATOM 7866 O GLU 1152 -23.867 -33.895 7.051 1.00 34.76 ATOM 7866 O GLU 1152 -24.942 -33.456 6.640 1.00 34.67 ATOM 7867 N SER 1153 -23.709 -35.147 7.468 1.00 34.67 ATOM 7868 CA SER 1153 -24.814 -36.102 7.456 1.00 34.62 ATOM 7869 CB SER 1153 -24.814 -36.102 7.456 1.00 34.62 ATOM 7870 OG SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7871 C SER 1153 -22.645 -37.926 6.357 1.00 39.86 ATOM 7872 O SER 1153 -25.787 -35.852 8.596 1.00 32.97 ATOM 7873 N GLY 1154 -26.30 -35.039 10.835 1.00 22.97 ATOM 7874 CA GLY 1154 -25.280 -35.039 10.835 1.00 28.64 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.31 ATOM 7878 CA VAL 1155 -224.944 -38.208 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -224.944 -38.208 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -224.944 -38.208 12.558 1.00 27.30 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 | | | | | | | | | |
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| ATOM 7859 CA GLU 1152 -22.637 -32.998 7.112 1.00 33.92 ATOM 7860 CB GLU 1152 -21.836 -33.117 5.813 1.00 34.31 ATOM 7861 CG GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7862 CD GLU 1152 -22.641 -32.774 4.567 1.00 38.13 ATOM 7863 OE1 GLU 1152 -22.337 -32.545 3.345 1.00 39.92 ATOM 7864 OE2 GLU 1152 -22.337 -32.491 2.240 1.00 43.20 ATOM 7865 C GLU 1152 -20.535 -32.498 3.485 1.00 41.00 ATOM 7866 O GLU 1152 -23.867 -33.895 7.051 1.00 34.76 ATOM 7866 O GLU 1152 -24.942 -33.456 6.640 1.00 35.70 ATOM 7867 N SER 1153 -23.709 -35.147 7.468 1.00 34.67 ATOM 7868 CA SER 1153 -24.814 -36.102 7.456 1.00 34.62 ATOM 7869 CB SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7870 OG SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7871 C SER 1153 -23.645 -37.926 6.357 1.00 39.86 ATOM 7872 O SER 1153 -225.787 -35.852 8.596 1.00 32.97 ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7876 C GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.31 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.21 ATOM 7878 CA VAL 1155 -24.944 -38.208 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -224.944 -38.208 12.558 1.00 27.30 ATOM 7870 CG VAL 1155 -224.944 -38.208 12.558 1.00 27.30 ATOM 7870 CG VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7878 CB VAL 1155 -23.728 -40.357 13.005 1.00 30.23 | | | | | | | | | |
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| ATOM 7862 CD GLU 1152 -21.775 -32.545 3.345 1.00 39.92 ATOM 7863 OE1 GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7864 OE2 GLU 1152 -20.535 -32.498 3.485 1.00 41.00 ATOM 7865 C GLU 1152 -23.867 -33.895 7.051 1.00 34.76 ATOM 7866 O GLU 1152 -24.942 -33.456 6.640 1.00 35.70 ATOM 7867 N SER 1153 -23.709 -35.147 7.468 1.00 34.67 ATOM 7868 CA SER 1153 -24.814 -36.102 7.456 1.00 34.62 ATOM 7869 CB SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7870 OG SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7871 C SER 1153 -23.645 -37.926 6.357 1.00 39.86 ATOM 7872 O SER 1153 -25.787 -35.852 8.596 1.00 32.97 ATOM 7873 N GLY 1154 -26.130 -35.039 10.835 1.00 32.97 ATOM 7874 CA GLY 1154 -26.130 -35.039 10.835 1.00 28.64 ATOM 7875 C GLY 1154 -26.130 -35.039 10.835 1.00 27.31 ATOM 7876 O GLY 1154 -26.491 -35.960 13.008 1.00 27.96 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.31 ATOM 7878 CA VAL 1155 -24.944 -38.208 12.558 1.00 27.30 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 | | | CB | | | -21.836 | -33.117 | 5.813 | 1.00 34.31 |
| ATOM 7863 OE1 GLU 1152 -22.337 -32.401 2.240 1.00 43.20 ATOM 7864 OE2 GLU 1152 -20.535 -32.498 3.485 1.00 41.00 ATOM 7865 C GLU 1152 -23.867 -33.895 7.051 1.00 34.76 ATOM 7866 O GLU 1152 -24.942 -33.456 6.640 1.00 35.70 ATOM 7867 N SER 1153 -23.709 -35.147 7.468 1.00 34.67 ATOM 7868 CA SER 1153 -24.814 -36.102 7.456 1.00 34.62 ATOM 7870 OG SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7870 OG SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7871 C SER 1153 -25.787 -35.852 8.596 1.00 32.97 ATOM 7872 O SER 1153 -26.974 -36.157 8.487 1.00 32.97 ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7874 CA GLY 1154 -26.130 -35.302 9.692 1.00 30.02 ATOM 7876 O GLY 1154 -26.130 -35.039 10.835 1.00 28.64 ATOM 7876 O GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7876 O GLY 1154 -26.491 -35.960 13.008 1.00 27.96 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.31 ATOM 7878 CA VAL 1155 -224.944 -38.208 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -24.944 -38.208 12.558 1.00 27.30 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7881 CG2 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 | MOTA | 7861 | CG | GLU | 1152 | -22.641 | -32.774 | 4.567 | 1.00 38.13 |
| ATOM 7864 OE2 GLU 1152 -20.535 -32.498 3.485 1.00 41.00 ATOM 7865 C GLU 1152 -23.867 -33.895 7.051 1.00 34.76 ATOM 7866 O GLU 1152 -24.942 -33.456 6.640 1.00 35.70 ATOM 7867 N SER 1153 -23.709 -35.147 7.468 1.00 34.67 ATOM 7869 CB SER 1153 -24.814 -36.102 7.456 1.00 34.62 ATOM 7870 OG SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7871 C SER 1153 -23.645 -37.926 6.357 1.00 39.86 ATOM 7872 O SER 1153 -25.787 -35.852 8.596 1.00 32.97 ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7875 C GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7876 O GLY 1154 -26.130 -35.039 10.835 1.00 28.64 ATOM 7876 O GLY 1154 -26.491 -35.960 13.008 1.00 27.31 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.21 ATOM 7878 CA VAL 1155 -24.944 -38.208 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -24.944 -38.208 12.558 1.00 27.30 ATOM 7878 CG VAL 1155 -224.944 -38.208 12.558 1.00 27.30 ATOM 7878 CG VAL 1155 -224.944 -38.208 12.558 1.00 27.30 ATOM 7878 CG VAL 1155 -224.944 -38.208 12.558 1.00 27.30 ATOM 7878 CG VAL 1155 -224.944 -38.208 12.558 1.00 27.30 ATOM 7878 CG VAL 1155 -224.944 -38.208 12.558 1.00 27.30 ATOM 7878 CG VAL 1155 -224.944 -38.208 12.558 1.00 27.30 ATOM 7878 CG VAL 1155 -224.944 -38.208 12.558 1.00 27.30 ATOM 7878 CG VAL 1155 -224.944 -38.208 12.558 1.00 27.30 ATOM 7880 CG1 VAL 1155 -224.924 -33.208 12.558 1.00 27.30 ATOM 7881 CG2 VAL 1155 -224.528 -39.828 10.692 1.00 31.88 | ATOM | 7862 | CD | GLU | 1152 | -21.775 | -32.545 | 3.345 | 1.00 39.92 |
| ATOM 7865 C GLU 1152 -23.867 -33.895 7.051 1.00 34.76 ATOM 7866 O GLU 1152 -24.942 -33.456 6.640 1.00 35.70 ATOM 7867 N SER 1153 -23.709 -35.147 7.468 1.00 34.67 ATOM 7868 CA SER 1153 -24.814 -36.102 7.456 1.00 34.62 ATOM 7869 CB SER 1153 -24.814 -37.544 7.559 1.00 35.72 ATOM 7870 OG SER 1153 -23.645 -37.926 6.357 1.00 39.86 ATOM 7871 C SER 1153 -25.787 -35.852 8.596 1.00 32.97 ATOM 7872 O SER 1153 -26.974 -36.157 8.487 1.00 33.54 ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7875 C GLY 1154 -26.130 -35.309 10.835 1.00 28.64 ATOM 7876 O GLY 1154 -26.430 -35.960 13.008 1.00 27.31 ATOM 7877 N VAL 1155 -25.952 -36.090 11.912 1.00 27.31 ATOM 7878 CA VAL 1155 -24.944 -38.208 12.558 1.00 27.32 ATOM 7878 CB VAL 1155 -23.969 -39.252 11.984 1.00 27.92 ATOM 7880 CG1 VAL 1155 -23.969 -39.252 11.984 1.00 27.92 ATOM 7881 CG2 VAL 1155 -24.528 -39.828 10.692 1.00 31.88 | ATOM | 7863 | OE1 | GLU | 1152 | -22.337 | -32.401 | 2.240 | 1.00 43.20 |
| ATOM 7866 O GLU 1152 -24.942 -33.456 6.640 1.00 35.70 ATOM 7867 N SER 1153 -23.709 -35.147 7.468 1.00 34.67 ATOM 7868 CA SER 1153 -24.814 -36.102 7.456 1.00 34.62 ATOM 7869 CB SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7870 OG SER 1153 -23.645 -37.926 6.357 1.00 39.86 ATOM 7871 C SER 1153 -25.787 -35.852 8.596 1.00 32.97 ATOM 7872 O SER 1153 -26.974 -36.157 8.487 1.00 33.54 ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7874 CA GLY 1154 -26.130 -35.039 10.835 1.00 28.64 ATOM 7875 C GLY 1154 -26.130 -35.039 10.835 1.00 28.64 ATOM 7876 O GLY 1154 -25.952 -36.090 11.912 1.00 27.31 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.21 ATOM 7878 CA VAL 1155 -22.969 -39.282 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -23.969 -39.828 10.692 1.00 30.23 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 | ATOM | 7864 | OE2 | GLU | 1152 | -20.535 | -32.498 | | 1.00 41.00 |
| ATOM 7867 N SER 1153 -23.709 -35.147 7.468 1.00 34.67 ATOM 7868 CA SER 1153 -24.814 -36.102 7.456 1.00 34.62 ATOM 7869 CB SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7870 OG SER 1153 -23.645 -37.926 6.357 1.00 39.86 ATOM 7871 C SER 1153 -25.787 -35.852 8.596 1.00 32.97 ATOM 7872 O SER 1153 -26.977 -36.157 8.487 1.00 33.54 ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7874 CA GLY 1154 -26.130 -35.039 10.835 1.00 28.64 ATOM 7875 C GLY 1154 -26.130 -35.039 10.835 1.00 28.64 ATOM 7876 O GLY 1154 -26.491 -35.960 13.008 1.00 27.91 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.21 ATOM 7878 CA VAL 1155 -24.944 -38.208 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 | ATOM | | С | | | | | | |
| ATOM 7868 CA SER 1153 -24.814 -36.102 7.456 1.00 34.62 ATOM 7869 CB SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7870 OG SER 1153 -23.645 -37.926 6.357 1.00 39.86 ATOM 7871 C SER 1153 -25.787 -35.852 8.596 1.00 32.97 ATOM 7872 O SER 1153 -26.974 -36.157 8.487 1.00 33.54 ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7874 CA GLY 1154 -26.130 -35.039 10.835 1.00 28.64 ATOM 7875 C GLY 1154 -26.130 -35.039 10.835 1.00 28.64 ATOM 7876 O GLY 1154 -25.952 -36.090 11.912 1.00 27.31 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.21 ATOM 7878 CA VAL 1155 -24.944 -38.208 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -23.969 -39.252 11.984 1.00 27.92 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7881 CG2 VAL 1155 -24.528 -39.828 10.692 1.00 31.88 | | | 0 | | | | | | |
| ATOM 7869 CB SER 1153 -24.284 -37.534 7.559 1.00 35.72 ATOM 7870 OG SER 1153 -23.645 -37.926 6.357 1.00 39.86 ATOM 7871 C SER 1153 -25.787 -35.852 8.596 1.00 32.97 ATOM 7872 O SER 1153 -26.974 -36.157 8.487 1.00 33.54 ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7874 CA GLY 1154 -26.130 -35.039 10.835 1.00 28.64 ATOM 7875 C GLY 1154 -25.952 -36.090 11.912 1.00 27.31 ATOM 7876 O GLY 1154 -26.491 -35.960 13.008 1.00 27.96 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.21 ATOM 7878 CA VAL 1155 -24.944 -38.208 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -23.768 -39.828 10.692 1.00 30.23 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 | | | | | | | | | |
| ATOM 7870 OG SER 1153 -23.645 -37.926 6.357 1.00 39.86 ATOM 7871 C SER 1153 -25.787 -35.852 8.596 1.00 32.97 ATOM 7872 O SER 1153 -26.974 -36.157 8.487 1.00 33.54 ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7875 C GLY 1154 -26.130 -35.039 10.835 1.00 28.64 ATOM 7876 O GLY 1154 -26.491 -35.960 13.008 1.00 27.31 ATOM 7876 N VAL 1155 -25.197 -37.140 11.599 1.00 27.21 ATOM 7878 CA VAL 1155 -24.944 -38.208 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -23.728 -40.357 13.005 1.00 27.92 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7881 CG2 VAL 1155 -24.528 -39.828 10.692 1.00 31.88 | | | | | | | | | |
| ATOM 7871 C SER 1153 -25.787 -35.852 8.596 1.00 32.97 ATOM 7872 O SER 1153 -26.974 -36.157 8.487 1.00 33.54 ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7874 CA GLY 1154 -26.130 -35.039 10.835 1.00 28.64 ATOM 7875 C GLY 1154 -26.130 -35.039 10.835 1.00 27.31 ATOM 7876 O GLY 1154 -26.491 -35.960 13.008 1.00 27.96 ATOM 7877 N VAL 1155 -26.491 -35.960 13.008 1.00 27.91 ATOM 7878 CA VAL 1155 -24.944 -38.208 12.558 1.00 27.21 ATOM 7879 CB VAL 1155 -23.969 -39.252 11.984 1.00 27.92 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7881 CG2 VAL 1155 -24.528 -39.828 10.692 1.00 31.88 | | | | | | | | | |
| ATOM 7872 O SER 1153 -26.974 -36.157 8.487 1.00 33.54 ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7874 CA GLY 1154 -26.130 -35.039 10.835 1.00 28.64 ATOM 7875 C GLY 1154 -26.952 -36.090 11.912 1.00 27.31 ATOM 7876 O GLY 1154 -26.491 -35.960 13.008 1.00 27.96 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.21 ATOM 7878 CA VAL 1155 -24.944 -38.208 12.558 1.00 27.20 ATOM 7879 CB VAL 1155 -23.969 -39.252 11.984 1.00 27.92 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7881 CG2 VAL 1155 -24.528 -39.828 10.692 1.00 31.88 | | | | | | | | | |
| ATOM 7873 N GLY 1154 -25.280 -35.302 9.692 1.00 30.02 ATOM 7874 CA GLY 1154 -26.130 -35.039 10.835 1.00 28.64 ATOM 7875 C GLY 1154 -25.952 -36.090 11.912 1.00 27.31 ATOM 7876 O GLY 1154 -26.491 -35.960 13.008 1.00 27.96 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.21 ATOM 7878 CA VAL 1155 -24.944 -38.208 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -23.969 -39.252 11.984 1.00 27.92 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7881 CG2 VAL 1155 -24.528 -39.828 10.692 1.00 31.88 | | | | | | | | | |
| ATOM 7874 CA GLY 1154 -26.130 -35.039 10.835 1.00 28.64 ATOM 7875 C GLY 1154 -25.952 -36.090 11.912 1.00 27.31 ATOM 7876 O GLY 1154 -26.491 -35.960 13.008 1.00 27.96 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.21 ATOM 7878 CA VAL 1155 -24.944 -38.208 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -23.969 -39.252 11.984 1.00 27.92 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7881 CG2 VAL 1155 -24.528 -39.828 10.692 1.00 31.88 | | | | | | | | | |
| ATOM 7875 C GLY 1154 -25.952 -36.090 11.912 1.00 27.31 ATOM 7876 O GLY 1154 -26.491 -35.960 13.008 1.00 27.96 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.21 ATOM 7878 CA VAL 1155 -24.944 -38.208 12.558 1.00 27.30 ATOM 7880 CG1 VAL 1155 -23.969 -39.252 11.984 1.00 27.92 ATOM 7881 CG2 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7881 CG2 VAL 1155 -24.528 -39.828 10.692 1.00 31.88 | | | | | | | | | |
| ATOM 7876 O GLY 1154 -26.491 -35.960 13.008 1.00 27.96 ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.21 ATOM 7878 CA VAL 1155 -24.944 -38.208 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -23.969 -39.252 11.984 1.00 27.92 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7881 CG2 VAL 1155 -24.528 -39.828 10.692 1.00 31.88 | | | | | | | | | |
| ATOM 7877 N VAL 1155 -25.197 -37.140 11.599 1.00 27.21 ATOM 7878 CA VAL 1155 -24.944 -38.208 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -23.969 -39.252 11.984 1.00 27.92 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7881 CG2 VAL 1155 -24.528 -39.828 10.692 1.00 31.88 | | | | | | | | | |
| ATOM 7878 CA VAL 1155 -24.944 -38.208 12.558 1.00 27.30 ATOM 7879 CB VAL 1155 -23.969 -39.252 11.984 1.00 27.92 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7881 CG2 VAL 1155 -24.528 -39.828 10.692 1.00 31.88 | | | | | | | | | |
| ATOM 7879 CB VAL 1155 -23.969 -39.252 11.984 1.00 27.92 ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7881 CG2 VAL 1155 -24.528 -39.828 10.692 1.00 31.88 | | | | | | | | | |
| ATOM 7880 CG1 VAL 1155 -23.728 -40.357 13.005 1.00 30.23 ATOM 7881 CG2 VAL 1155 -24.528 -39.828 10.692 1.00 31.88 | | | | | | | | | |
| ATOM 7881 CG2 VAL 1155 -24.528 -39.828 10.692 1.00 31.88 | | | | | | | | | |
| | | | | | | | | | |
| | | | | | | | | 13.823 | 1.00 26.47 |

| ATOM | 7883 | 0 | VAL | 1155 | | -24.616 | -38.065 | 14.935 | 1.00 26.28 |
|--------------|------|-----|-----|------|-----|---------|--------------------|------------------|--------------------------|
| ATOM | 7884 | N | TYR | 1156 | | -23.485 | -36.606 | 13.636 | 1.00 25.70 |
| MOTA | 7885 | CA | TYR | 1156 | | -22.828 | -35.921 | 14.746 | 1.00 25.82 |
| MOTA | 7886 | CB | TYR | 1156 | | -21.307 | -36.124 | 14.709 | 1.00 24.74 |
| MOTA | 7887 | CG | TYR | 1156 | | -20.605 | -35.437 | 15.867 | 1.00 24.07 |
| ATOM | 7888 | CD1 | TYR | 1156 | | -20.649 | -35.976 | 17.156 | 1.00 23.28 |
| ATOM | 7889 | CE1 | TYR | 1156 | | -20.078 | -35.306 | 18.242 | 1.00 23.96 |
| MOTA | 7890 | CD2 | TYR | 1156 | | -19.964 | -34.213 | 15.690 | 1.00 24.41 |
| ATOM | 7891 | CE2 | TYR | 1156 | | -19.392 | -33.533 | 16.768 | 1.00 24.50 |
| ATOM | 7892 | CZ | TYR | 1156 | | -19.455 | -34.083 | 18.041 | 1.00 24.23 |
| ATOM | 7893 | ОН | TYR | 1156 | | -18.920 | -33.395 | 19.112 | 1.00 23.15 |
| ATOM | 7894 | С | TYR | 1156 | | -23.116 | -34.424 | 14.696 | 1.00 26.27 |
| MOTA | 7895 | 0 | TYR | 1156 | | -22.996 | -33.799 | 13.642 | 1.00 26.36 |
| MOTA | 7896 | N | PRO | 1157 | | -23.471 | -33.826 | 15.844 | 1.00 27.37 |
| ATOM | 7897 | CD | PRO | 1157 | | -23.555 | -32.365 | 16.017 | 1.00 28.85 |
| ATOM | 7898 | CA | PRO | 1157 | | -23.600 | -34.509 | 17.132 | 1.00 28.73 |
| ATOM | 7899 | CB | PRO | 1157 | | -23.499 | -33.365 | 18.138 | 1.00 28.98 |
| MOTA | 7900 | CG | PRO | 1157 | | -24.117 | -32.234 | 17.416 | 1.00 29.31 |
| ATOM | 7901 | С | PRO | 1157 | | -24.882 | -35.319 | 17.290 | 1.00 30.00 |
| ATOM | 7902 | 0 | PRO | 1157 | | -25.928 | -34.970 | 16.740 | 1.00 29.72 |
| MOTA | 7903 | N | GLY | 1158 | | -24.786 | -36.409 | 18.046 | 1.00 30.34 |
| MOTA | 7904 | CA | GLY | 1158 | | -25.940 | -37.257 | 18.278 | 1.00 31.69 |
| ATOM | 7905 | С | GLY | 1158 | | -26.668 | -36.843 | 19.540 | 1.00 32.83 |
| ATOM | 7906 | 0 | GLY | 1158 | | -26.240 | -35.921 | 20.234 | 1.00 31.48 |
| MOTA | 7907 | N | GLU | 1159 | | -27.770 | -37.521 | 19.844 | 1.00 33.48 |
| ATOM | 7908 | CA | GLU | 1159 | | -28.538 | -37.198 | 21.036 | 1.00 34.89 |
| ATOM | 7909 | CB | GLU | 1159 | | -29.791 | -38.075 | 21.122 | 1.00 36.68 |
| ATOM | 7910 | CG | GLU | 1159 | | -30.853 | -37.515 | 22.049 | 1.00 38.05 |
| ATOM | 7911 | CD | GLU | 1159 | | -31.472 | -36.241 | 21.503 | 1.00 39.50 |
| MOTA | 7912 | OE1 | GLU | 1159 | | -32.152 | -35.527 | 22.269 | 1.00 41.54 |
| ATOM | 7913 | OE2 | GLU | 1159 | | -31.282 | -35.958 | 20.300 | 1.00 39.55 |
| MOTA | 7914 | С | GLU | 1159 | | -27.685 | -37.403 | 22.283 | 1.00 35.20 |
| ATOM | 7915 | 0 | GLU | 1159 | | -27.943 | -36.802 | 23.325 | 1.00 35.87 |
| ATOM | 7916 | N | GLU | 1160 | | -26.668 | -38.256 | 22.167 | 1.00 35.14 |
| ATOM | 7917 | CA | GLU | 1160 | | -25.764 | -38.545 | 23.277 | 1.00 35.10 |
| MOTA | 7918 | CB | GLU | 1160 | | -24.870 | -39.748 | 22.951 | 1.00 37.43 |
| MOTA | 7919 | CG | GLU | 1160 | | -25.577 | -40.902 | 22.261 | 1.00 41.76 |
| MOTA | 7920 | CD | GLU | 1160 | | -25.822 | -40.638 | 20.789 | 1.00 42.93 |
| MOTA | 7921 | OE1 | GLU | 1160 | | -24.834 | -40.410 | 20.054 | 1.00 43.83 |
| MOTA | 7922 | OE2 | GLU | 1160 | | -26.999 | -40.666 | 20.368 | 1.00 43.38 |
| MOTA | 7923 | С | GLU | 1160 | | -24.862 | -37.353 | 23.583 | 1.00 33.30 |
| ATOM | 7924 | 0 | GLU | 1160 | | -24.259 | -37.285 | 24.654 | 1.00 31.07 |
| MOTA | 7925 | N | HIS | 1161 | | -24.777 | -36.422 | 22.637 | 1.00 32.51 |
| MOTA | 7926 | CA | HIS | 1161 | | -23.930 | -35.238 | 22.781 | 1.00 32.09 |
| MOTA | 7927 | CB | HIS | 1161 | | -23.016 | -35.097 | 21.562 | 1.00 31.02 |
| MOTA | 7928 | CG | HIS | 1161 | | -22.355 | -36.373 | 21.143 | 1.00 29.12 |
| MOTA | 7929 | | HIS | 1161 | | -22.512 | -37.131 | 20.032 | 1.00 27.73 |
| MOTA | 7930 | ND1 | HIS | 1161 | | -21.407 | -37.013 | 21.913 | 1.00 28.00 |
| MOTA | 7931 | CE1 | HIS | 1161 | | -21.012 | -38.112 | 21.296 | 1.00 27.95 |
| MOTA | 7932 | NE2 | HIS | 1161 | | -21.667 | -38.207 | 20.152 | 1.00 29.03 |
| ATOM | 7933 | С | HIS | 1161 | | -24.757 | -33.965 | 22.899 | 1.00 33.71 |
| MOTA | 7934 | 0 | HIS | 1161 | | | -32.864 | 22.874 | 1.00 31.48 |
| MOTA | 7935 | N | SER | 1162 | | | -34.121 | 23.028 | 1.00 34.90 |
| ATOM | 7936 | CA | SER | 1162 | | -26.969 | -32.981 | 23.107 | 1.00 36.32 |
| ATOM | 7937 | CB | SER | 1162 | | -28.088 | -33.167 | 22.088 | 1.00 36.36 |
| MOTA | 7938 | OG | SER | 1162 | | -27.543 | -33.422 | 20.806 | 1.00 37.50 |
| MOTA | 7939 | С | SER | 1162 | | -27.562 | -32.748 | 24.492 | 1.00 37.54 |
| MOTA | 7940 | 0 | SER | 1162 | | -27.649 | -33.670 | 25.303 | 1.00 37.53 |
| MOTA | 7941 | N | PHE | 1163 | | -27.969 | -31.505 | 24.749 | 1.00 38.51 |
| MOTA | 7942 | CA | PHE | 1163 | | -28.563 | -31.129 | 26.028 | 1.00 39.57 |
| MOTA | 7943 | CB | PHE | 1163 | | -27.764 | -30.000 | 26.692 | 1.00 40.57 |
| ATOM | 7944 | CG | PHE | 1163 | | -26.323 | -30.346 | 26.967 | 1.00 43.95 |
| MOTA | 7945 | CD1 | | 1163 | | -25.363 | -30.253 | 25.961 | 1.00 44.75 |
| MOTA | 7946 | | PHE | 1163 | | -25.926 | -30.771 | 28.232 | 1.00 44.14 |
| ATOM | 7947 | CE1 | | 1163 | | | -30.575 | 26.213 | 1.00 45.36 |
| ATOM | 7948 | CE2 | | 1163 | | | | 28.492 | 1.00 45.59 |
| ATOM | 7949 | CZ | PHE | 1163 | . ' | -23.645 | -30.998 | 27.480 | 1.00 44.94 |
| ATOM | 7950 | C | PHE | 1163 | | -30.007 | -30.676 | 25.838 | 1.00 39.51 |
| ATOM | 7951 | 0 | PHE | 1163 | | -30.449 | -30.433 | 24.715 | 1.00 39.54 |
| ATOM | 7952 | N | HIS | 1164 | | | -30.562 | 26.944 | 1.00 40.34 |
| ATOM | 7953 | CA | HIS | 1164 | | -32.132 | -30.136 | 26.912 | 1.00 40.45 |
| MOTA | 7954 | CB | HIS | 1164 | | -33.056 | -31.351 | 26.812 | 1.00 39.13 |
| ATOM | 7955 | CG | HIS | 1164 | | -32.963 | -32.071 | 25.504 | 1.00 37.46 |
| ATOM | 7956 | | HIS | 1164 | | -32.563 | -33.329 | 25.201 | 1.00 36.29 1.00 36.11 |
| ATOM | 7957 | | HIS | 1164 | | -33.293 | -31.476 | 24.305 23.321 | 1.00 36.11 |
| ATOM ATOM | 7958 | | HIS | 1164 | | | -32.336 -33.468 | 23.321 | 1.00 34.87 |
| ATOM | 7959 | NEZ | HIS | 1164 | | -34.03/ | -33.400 | 23.05 (| 1.00 24.03 |

| ATOM | 7960 | С | HIS | 1164 | -32.484 | -29.320 | 28.149 | 1.00 41.45 |
|------|------|-----|-----|------|---------|---------|--------|------------|
| ATOM | 7961 | 0 | HIS | 1164 | -33.130 | -28.261 | 27.988 | 1.00 42.79 |
| ATOM | 7962 | ОХТ | HIS | 1164 | -32.118 | -29.749 | 29.264 | 1.00 42.44 |
| ATOM | 7963 | C1 | KPL | 1165 | -14.350 | -24.823 | 22.600 | 1.00 37.46 |
| ATOM | 7964 | C2 | KPL | 1165 | | -23.614 | 21.664 | 1.00 35.76 |
| ATOM | 7965 | C3 | KPL | 1165 | | -24.044 | 20.219 | 1.00 36.86 |
| ATOM | 7966 | C4 | KPL | 1165 | | -23.142 | 21.763 | 1.00 37.77 |
| ATOM | 7967 | 01 | KPL | 1165 | | -22.744 | 23.112 | 1.00 39.26 |
| | | | | | | -22.469 | 22.059 | 1.00 34.45 |
| ATOM | 7968 | C5 | KPL | 1165 | | | | |
| ATOM | 7969 | 02 | KPL | 1165 | | -21.380 | 22.384 | 1.00 34.78 |
| MOTA | 7970 | C6 | KPL | 1165 | | -22.661 | 22.058 | 1.00 32.52 |
| MOTA | 7971 | 03 | KPL | 1165 | | -23.720 | 21.736 | 1.00 31.95 |
| MOTA | 7972 | 04 | KPL | 1165 | | -21.651 | 22.419 | 1.00 28.43 |
| MOTA | 7973 | CB | MET | 1201 | | -28.638 | 47.750 | 1.00 74.61 |
| MOTA | 7974 | CG | MET | 1201 | -16.080 | -29.937 | 48.288 | 1.00 76.04 |
| MOTA | 7975 | SD | MET | 1201 | -15.715 | -31.415 | 47.313 | 1.00 77.75 |
| ATOM | 7976 | CE | MET | 1201 | -17.296 | -31.664 | 46.480 | 1.00 77.07 |
| ATOM | 7977 | С | MET | 1201 | -15.060 | -28.920 | 45.290 | 1.00 71.84 |
| ATOM | 7978 | 0 | MET | 1201 | -13.988 | -29.442 | 45.601 | 1.00 72.20 |
| ATOM | 7979 | N | MET | 1201 | -17.380 | -28.524 | 46.164 | 1.00 73.50 |
| ATOM | 7980 | CA | MET | 1201 | | -28.231 | 46.340 | 1.00 73.03 |
| ATOM | 7981 | N | LYS | 1202 | | -28.905 | 44.043 | 1.00 69.78 |
| ATOM | 7982 | CA | LYS | 1202 | | -29.524 | 42.940 | 1.00 67.53 |
| ATOM | 7983 | CB | LYS | 1202 | | -30.791 | 42.469 | 1.00 68.57 |
| | | | | 1202 | | -31.977 | | 1.00 69.98 |
| ATOM | 7984 | CG | LYS | | | | 43.422 | |
| ATOM | 7985 | CD | LYS | 1202 | | -32.611 | 43.409 | 1.00 70.39 |
| ATOM | 7986 | CE | LYS | 1202 | -13.781 | | 42.140 | 1.00 70.57 |
| ATOM | 7987 | NZ | LYS | 1202 | -13.778 | | 40.895 | 1.00 70.61 |
| ATOM | 7988 | C | LYS | 1202 | | -28.580 | 41.752 | 1.00 64.73 |
| ATOM | 7989 | 0 | LYS | 1202 | -15.029 | -28.890 | 40.637 | 1.00 65.32 |
| ATOM | 7990 | N | PRO | 1203 | -13.973 | -27.414 | 41.973 | 1.00 61.55 |
| ATOM | 7991 | CD | PRO | 1203 | -13.472 | -26.591 | 40.856 | 1.00 60.49 |
| ATOM | 7992 | CA | PRO | 1203 | -13.433 | -26.929 | 43.248 | 1.00 58.33 |
| ATOM | 7993 | CB | PRO | 1203 | -12.232 | -26.108 | 42.802 | 1.00 58.95 |
| ATOM | 7994 | CG | PRO | 1203 | | -25.453 | 41.571 | 1.00 59.90 |
| ATOM | 7995 | C | PRO | 1203 | | -26.086 | 44.018 | 1.00 55.17 |
| ATOM | 7996 | o | PRO | 1203 | | -26.081 | 43.689 | 1.00 55.08 |
| | | | | 1203 | | -25.372 | 45.039 | 1.00 50.88 |
| ATOM | 7997 | N | THR | | | | | |
| ATOM | 7998 | CA | THR | 1204 | -14.863 | | 45.843 | 1.00 46.61 |
| ATOM | 7999 | CB | THR | 1204 | | -24.061 | 47.140 | 1.00 46.19 |
| MOTA | 8000 | OG1 | | 1204 | | -25.204 | 47.870 | 1.00 46.22 |
| MOTA | 8001 | CG2 | THR | 1204 | | -23.273 | 48.009 | 1.00 45.19 |
| ATOM | 8002 | С | THR | 1204 | | -23.288 | 45.026 | 1.00 43.63 |
| MOTA | 8003 | 0 | THR | 1204 | | -22.642 | 44.440 | 1.00 42.49 |
| MOTA | 8004 | N | THR | 1205 | -16.531 | -22.966 | 44.985 | 1.00 40.26 |
| MOTA | 8005 | CA | THR | 1205 | -17.000 | -21.811 | 44.222 | 1.00 37.82 |
| MOTA | 8006 | CB | THR | 1205 | -17.760 | -22.241 | 42.953 | 1.00 38.23 |
| MOTA | 8007 | OG1 | THR | 1205 | -18.955 | -22.937 | 43.330 | 1.00 39.06 |
| MOTA | 8008 | CG2 | THR | 1205 | -16.893 | -23.142 | 42.089 | 1.00 39.20 |
| ATOM | 8009 | С | THR | 1205 | -17.924 | -20.887 | 45.002 | 1.00 35.47 |
| ATOM | 8010 | ō | THR | 1205 | | -21.201 | 46.111 | 1.00 34.25 |
| ATOM | 8011 | N | ILE | 1206 | | -19.744 | 44.397 | 1.00 33.47 |
| ATOM | 8012 | CA | ILE | 1206 | | -18.761 | 45.010 | 1.00 34.02 |
| ATOM | 8013 | CB | ILE | 1206 | | -17.528 | 44.107 | 1.00 34.29 |
| | | | | | | -16.455 | 44.834 | 1.00 34.25 |
| MOTA | 8014 | CG2 | ILE | 1206 | | | | |
| ATOM | 8015 | CG1 | ILE | 1206 | | -16.986 | 43.728 | 1.00 36.56 |
| ATOM | 8016 | CD1 | | 1206 | -17.908 | -15.950 | 42.616 | 1.00 36.92 |
| MOTA | 8017 | С | ILE | 1206 | -20.481 | -19.368 | 45.266 | 1.00 33.47 |
| MOTA | 8018 | 0 | ILE | 1206 | -21.119 | -19.080 | 46.280 | 1.00 33.95 |
| MOTA | 8019 | N | SER | 1207 | -20.933 | -20.218 | 44.350 | 1.00 33.47 |
| MOTA | 8020 | CA | SER | 1207 | -22.236 | -20.861 | 44.494 | 1.00 34.07 |
| MOTA | 8021 | CB | SER | 1207 | -22.515 | -21.766 | 43.292 | 1.00 34.94 |
| MOTA | 8022 | OG | SER | 1207 | -22.693 | -21.001 | 42.111 | 1.00 37.78 |
| MOTA | 8023 | С | SER | 1207 | -22.310 | | 45.777 | 1.00 33.33 |
| ATOM | 8024 | Ō | SER | 1207 | -23.392 | -21.899 | 46.319 | 1.00 34.33 |
| ATOM | 8025 | N | LEU | 1208 | -21.152 | -22.121 | 46.259 | 1.00 32.96 |
| ATOM | 8026 | CA | LEU | 1208 | -21.086 | -22.919 | 47.477 | 1.00 32.87 |
| ATOM | 8027 | CB | LEU | 1208 | -19.676 | | 47.651 | 1.00 32.07 |
| ATOM | 8027 | CG | LEU | 1208 | -19.539 | | 48.189 | 1.00 34.10 |
| | | | | | | | 48.489 | 1.00 35.32 |
| ATOM | 8029 | | LEU | 1208 | | -25.215 | | |
| MOTA | 8030 | | LEU | 1208 | | -25.092 | 49.440 | 1.00 34.02 |
| MOTA | 8031 | C | LEU | 1208 | -21.444 | -22.062 | 48.687 | 1.00 31.67 |
| MOTA | 8032 | 0 | LEU | 1208 | | -22.488 | 49.563 | 1.00 30.68 |
| MOTA | 8033 | N | LEU | 1209 | | -20.848 | 48.728 | 1.00 29.45 |
| MOTA | 8034 | CA | LEU | 1209 | | -19.934 | 49.834 | 1.00 28.92 |
| MOTA | 8035 | CB | LEU | 1209 | | -18.753 | 49.772 | 1.00 25.98 |
| MOTA | 8036 | CG | LEU | 1209 | -18.698 | -19.117 | 49.742 | 1.00 25.45 |
| | | | | | | | | |

| MOTA | 8037 | CD1 | LEU | 1209 | | -17.859 | -17.844 | 49.746 | 1.00 22.70 |
|--------|------|-----|-----|------|---|---------|---------|---------|------------|
| ATOM | 8038 | CD2 | LEU | 1209 | | -18.356 | -19.975 | 50.947 | 1.00 23.49 |
| ATOM | 8039 | C | LEU | 1209 | | | -19.425 | 49.802 | 1.00 29.02 |
| | | | | | | | | | |
| ATOM | 8040 | 0 | LEU | 1209 | | | -19.198 | 50.844 | 1.00 28.22 |
| ATOM | 8041 | N | GLN | 1210 | | -23.126 | -19.239 | 48.598 | 1.00 30.69 |
| ATOM | 8042 | CA | GLN | 1210 | | -24.497 | -18.763 | 48.436 | 1.00 32.68 |
| ATOM | 8043 | CB | GLN | 1210 | | | -18.499 | 46.954 | 1.00 32.40 |
| | | | | | | | | | |
| ATOM | 8044 | CG | GLN | 1210 | | | -17.885 | 46.648 | 1.00 33.66 |
| MOTA | 8045 | CD | GLN | 1210 | | -26.378 | -16.573 | 47.372 | 1.00 33.08 |
| ATOM | 8046 | OE1 | GLN | 1210 | | -26.857 | -16.553 | 48.506 | 1.00 33.39 |
| ATOM | 8047 | NE2 | GLN | 1210 | | | -15.467 | 46.722 | 1.00 31.00 |
| | | | | | | | | | |
| MOTA | 8048 | C | GLN | 1210 | | | -19.831 | 48.994 | 1.00 33.63 |
| ATOM | 8049 | 0 | GLN | 1210 | | -26.437 | -19.520 | 49.643 | 1.00 34.19 |
| MOTA | 8050 | N | LYS | 1211 | | -25.095 | -21.093 | 48.750 | 1.00 35.83 |
| ATOM | 8051 | CA | LYS | 1211 | | -25.888 | -22.212 | 49.247 | 1.00 37.75 |
| ATOM | 8052 | СВ | LYS | 1211 | | | -23.533 | 48.670 | 1.00 39.41 |
| | | | | | | | | | |
| MOTA | 8053 | CG | LYS | 1211 | | | -24.766 | 49.413 | 1.00 43.61 |
| MOTA | 8054 | CD | LYS | 1211 | | -25.471 | -26.064 | 48.717 | 1.00 46.26 |
| MOTA | 8055 | CE | LYS | 1211 | | -26.318 | -26.314 | 47.477 | 1.00 47.80 |
| MOTA | 8056 | NZ | LYS | 1211 | | -26.008 | -27.629 | 46.849 | 1.00 49.02 |
| | 8057 | C | LYS | 1211 | | -25.833 | | 50.775 | 1.00 38.19 |
| MOTA | | | | | | | | | |
| ATOM | 8058 | 0 | LYS | 1211 | | | -22.579 | 51.434 | 1.00 37.83 |
| MOTA | 8059 | N | TYR | 1212 | | -24.673 | -21.930 | 51.334 | 1.00 37.94 |
| MOTA | 8060 | CA | TYR | 1212 | | -24.493 | -21.933 | 52.781 | 1.00 38.24 |
| ATOM | 8061 | CB | TYR | 1212 | | -23.032 | | 53.128 | 1.00 39.33 |
| ATOM | 8062 | CG | TYR | 1212 | | -22.101 | | 52.936 | 1.00 41.48 |
| | | | | | • | | | | |
| MOTA | 8063 | | TYR | 1212 | | | -22.623 | 52.830 | 1.00 43.21 |
| MOTA | 8064 | CE1 | TYR | 1212 | | -19.854 | -23.698 | 52.690 | 1.00 44.20 |
| ATOM | 8065 | CD2 | TYR | 1212 | | -22.587 | -24.125 | 52.897 | 1.00 42.82 |
| ATOM | 8066 | CE2 | TYR | 1212 | | -21.724 | | 52.759 | 1.00 44.18 |
| | | | | | | | | | |
| ATOM | 8067 | CZ | TYR | 1212 | | | -24.987 | 52.657 | 1.00 44.87 |
| MOTA | 8068 | OH | TYR | 1212 | | -19.496 | -26.048 | 52.522 | 1.00 46.35 |
| MOTA | 8069 | С | TYR | 1212 | | -25.388 | -20.922 | 53.485 | 1.00 37.78 |
| ATOM | 8070 | 0 | TYR | 1212 | | -25.946 | -21.211 | 54.544 | 1.00 36.95 |
| | 8071 | N | LYS | 1213 | | | -19.731 | 52.906 | 1.00 37.50 |
| MOTA | | | | | | | | | |
| ATOM | 8072 | CA | LYS | 1213 | | -26.348 | | 53.506 | 1.00 37.53 |
| ATOM | 8073 | CB | LYS | 1213 | | -26.256 | -17.387 | 52.707 | 1.00 35.24 |
| MOTA | 8074 | CG | LYS | 1213 | | -27.168 | -16.292 | 53.248 | 1.00 31.66 |
| ATOM | 8075 | CD | LYS | 1213 | | | -14.894 | 52.831 | 1.00 27.83 |
| | | | | | | | | | 1.00 27.03 |
| ATOM | 8076 | CE | LYS | 1213 | | | -13.850 | 53.530 | |
| ATOM | 8077 | NZ | LYS | 1213 | | | -12.467 | 53.408 | 1.00 24.51 |
| MOTA | 8078 | C | LYS | 1213 | | -27.803 | -19.146 | 53.591 | 1.00 39.33 |
| ATOM | 8079 | 0 | LYS | 1213 | | -28.451 | -18.980 | 54.624 | 1.00 39.00 |
| MOTA | 8080 | N | GLN | 1214 | | | -19.717 | 52.505 | 1.00 40.82 |
| | | | | | | -29.689 | | 52.481 | 1.00 43.81 |
| MOTA | 8081 | CA | GLN | 1214 | | | | | |
| MOTA | 8082 | CB | GLN | 1214 | | | -20.692 | 51.084 | 1.00 45.23 |
| MOTA | 8083 | CG | GLN | 1214 | | -30.123 | -19.591 | 50.037 | 1.00 48.26 |
| ATOM | 8084 | CD | GLN | 1214 | | -30.583 | -20.097 | 48.684 | 1.00 50.37 |
| ATOM | 8085 | OE1 | GLN | 1214 | | -31.663 | -20.683 | 48.561 | 1.00 52.18 |
| ATOM | 8086 | NE2 | GLN | 1214 | | -29.767 | -19.870 | 47.656 | 1.00 50.33 |
| | | | | | - | | | | |
| MOTA | 8087 | С | GLN | 1214 | | -29.889 | | 53.501 | 1.00 44.29 |
| MOTA | 8808 | 0 | GLN | 1214 | | -30.948 | -21.406 | 54.118 | 1.00 44.96 |
| ATOM | 8089 | N | GLU | 1215 | | -28.862 | -22.126 | 53.683 | 1.00 45.06 |
| ATOM | 8090 | CA | GLU | 1215 | | -28.934 | -23.229 | 54.633 | 1.00 45.32 |
| ATOM | 8091 | CB | GLU | 1215 | | -27.960 | | 54.241 | 1.00 46.90 |
| | | | | | | | -24.843 | 52.815 | 1.00 49.76 |
| ATOM | 8092 | CG | GLU | 1215 | | | | | |
| MOTA | 8093 | CD | GLU | 1215 | | -27.175 | | 52.522 | 1.00 51.37 |
| ATOM | 8094 | OE1 | GLU | 1215 | | -25.983 | -25.927 | 52.888 | 1.00 52.64 |
| MOTA | 8095 | OE2 | GLU | 1215 | | -27.635 | -27.000 | 51.920 | 1.00 52.49 |
| ATOM | 8096 | C | GLU | 1215 | | | -22.744 | 56.036 | 1.00 44.97 |
| | | | | 1215 | | | -23.541 | 56.969 | 1.00 44.92 |
| MOTA | 8097 | 0 | GLU | | | | | | |
| MOTA | 8098 | N | LYS | 1216 | | -28.400 | | 56.182 | 1.00 44.76 |
| MOTA | 8099 | CA | LYS | 1216 | | -28.069 | | 57.479 | 1.00 43.95 |
| MOTA | 8100 | CB | LYS | 1216 | | -29.252 | -21.001 | 58.442 | 1.00 45.68 |
| ATOM | 8101 | CG | LYS | 1216 | | -30.481 | | 58.071 | 1.00 48.07 |
| ATOM | 8102 | CD | LYS | 1216 | | -30.234 | | 58.255 | 1.00 49.08 |
| | | | | | | | | | |
| ATOM | 8103 | CE | LYS | 1216 | | -31.475 | | 57.914 | 1.00 50.43 |
| MOTA | 8104 | NZ | LYS | 1216 | | -32.654 | | 58.740 | 1.00 51.79 |
| ATOM | 8105 | С | LYS | 1216 | | -26.829 | -21.509 | 58.085 | 1.00 42.80 |
| ATOM | 8106 | 0 | LYS | 1216 | | -26.763 | -21.741 | 59.296 | 1.00 42.94 |
| АТОМ | 8107 | N | LYS | 1217 | | -25.850 | -21.813 | 57.239 | 1.00 40.87 |
| | | | | | | | | 57.693 | |
| ATOM | 8108 | CA | LYS | 1217 | | -24.613 | -22.444 | | 1.00 39.09 |
| MOTA | 8109 | CB | LYS | 1217 | | -24.290 | -23.667 | 56.830 | 1.00 39.84 |
| MOTA | 8110 | CG | LYS | 1217 | | -22.929 | -24.284 | 57.143 | 1.00 42.69 |
| MOTA | 8111 | CD | LYS | 1217 | | -22.622 | -25.474 | 56.250 | 1.00 45.14 |
| ATOM | 8112 | CE | LYS | 1217 | | | -26.651 | 56.546 | 1.00 47.62 |
| ATOM | | | | | | -23.209 | | 55.706 | 1.00 48.86 |
| A I OM | 8113 | NZ | LYS | 1217 | | -23.209 | -21.638 | JJ. 100 | T.00 #0.00 |
| | | | | | | | | | |

| ATOM | 8114 | С | LYS | 1217 | -23.439 | -21.471 | 57.646 | 1.00 36.74 |
|------|--------------|--------|------------|--------------|---------|---------|--------|------------|
| ATOM | 8115 | 0 | LYS | 1217 | -22.930 | | 56.573 | 1.00 37.26 |
| ATOM | 8116 | N | ARG | 1218 | -23.008 | -21.003 | 58.812 | 1.00 33.47 |
| ATOM | 8117 | CA | ARG | 1218 | -21.892 | -20.069 | 58.890 | 1.00 31.52 |
| ATOM | 8118 | CB | ARG | 1218 | -21.799 | -19.498 | 60.309 | 1.00 32.55 |
| ATOM | 8119 | CG | ARG | 1218 | -22.894 | -18.476 | 60.603 | 1.00 31.60 |
| ATOM | 8120 | CD | ARG | 1218 | | -18.029 | 62.052 | 1.00 33.28 |
| ATOM | 8121 | NE | ARG | 1218 | -23.699 | -18.938 | 62.890 | 1.00 33.49 |
| ATOM | 8122 | CZ | ARG | 1218 | | -18.678 | 64.145 | 1.00 32.58 |
| ATOM | 8123 | NH1 | | 1218 | -23.688 | -17.537 | 64.716 | 1.00 33.26 |
| ATOM | 8124 | NH2 | | 1218 | -24.767 | -19.554 | 64.828 | 1.00 34.35 |
| ATOM | 8125 | С | ARG | 1218 | -20.578 | -20.737 | 58.476 | 1.00 30.31 |
| АТОМ | 8126 | Ō | ARG | 1218 | -20.223 | -21.797 | 58.990 | 1.00 31.64 |
| АТОМ | 8127 | N | PHE | 1219 | | -20.112 | 57.543 | 1.00 28.09 |
| ATOM | 8128 | CA | PHE | 1219 | -18.607 | | 57.038 | 1.00 24.32 |
| ATOM | 8129 | CB | PHE | 1219 | | -20.816 | 55.518 | 1.00 23.44 |
| ATOM | 8130 | CG | PHE | 1219 | -19.005 | -19.537 | 54.794 | 1.00 22.44 |
| ATOM | 8131 | CD1 | | 1219 | | -18.711 | 54.343 | 1.00 21.27 |
| ATOM | 8132 | CD2 | | 1219 | -20.321 | -19.131 | 54.606 | 1.00 22.38 |
| ATOM | 8133 | CE1 | | 1219 | -18.253 | -17.495 | 53.719 | 1.00 20.07 |
| ATOM | 8134 | CE2 | PHE | 1219 | | -17.918 | 53.983 | 1.00 20.42 |
| ATOM | 8135 | CZ | PHE | 1219 | -19.575 | | 53.539 | 1.00 22.14 |
| ATOM | 8136 | C | PHE | 1219 | | -19.811 | 57.411 | 1.00 24.16 |
| ATOM | 8137 | 0 | PHE | 1219 | -17.476 | | 57.576 | 1.00 20.50 |
| ATOM | 8138 | N | ALA | 1220 | -16.238 | | 57.541 | 1.00 23.05 |
| ATOM | 8139 | CA | ALA | 1220 | -14.992 | | 57.908 | 1.00 23.62 |
| ATOM | 8140 | CB | ALA | 1220 | -14.195 | | 58.867 | 1.00 23.36 |
| ATOM | 8141 | С | ALA | 1220 | -14.134 | | 56.698 | 1.00 20.64 |
| | | | | | -14.081 | | 55.729 | 1.00 20.76 |
| MOTA | 8142 8143 | O N | ALA THR | 1220 1221 | -13.462 | | 56.773 | 1.00 20.76 |
| ATOM | | | | | -12.593 | | 55.700 | 1.00 20.30 |
| ATOM | 8144 | CA | THR | 1221 | -12.393 | | 54.950 | 1.00 21.27 |
| ATOM | 8145 | CB | THR | 1221 1221 | | | 54.456 | 1.00 25.31 |
| ATOM | 8146 | OG1 | THR | | -14.532 | | | |
| MOTA | 8147 | CG2 | THR | 1221 | -12.391 | | 53.790 | 1.00 26.49 |
| | 8148 | C | THR | 1221 | -11.271 | | 56.329 | 1.00 20.19 |
| MOTA | 8149 | 0 | THR | 1221 | -11.225 | | 57.515 | 1.00 19.48 |
| MOTA | 8150 | N | ILE | 1222 | -10.192 | | 55.552 | 1.00 20.17 |
| MOTA | 8151 | CA | ILE | 1222 | | -16.975 | 56.129 | 1.00 18.40 |
| MOTA | 8152 | CB | ILE | 1222 | | -18.211 | 56.779 | 1.00 19.49 |
| MOTA | 8153 | CG2 | ILE | 1222 | | -19.105 | 55.696 | 1.00 20.26 |
| MOTA | 8154 | CG1 | ILE | 1222 | | -17.753 | 57.794 | 1.00 21.68 |
| ATOM | 8155 | CD1 | ILE | 1222 | | -18.886 | 58.621 | 1.00 25.50 |
| ATOM | 8156 | С | ILE | 1222 | | -16.338 | 55.115 | 1.00 18.20 |
| MOTA | 8157 | 0 | ILE | 1222 | | -16.510 | 53.910 | 1.00 17.49 |
| MOTA | 8158 | N | THR | 1223 | | -15.575 | 55.602 | 1.00 19.22 |
| ATOM | 8159 | CA | THR | 1223 | | -14.950 | 54.695 | 1.00 19.12 |
| MOTA | 8160 | CB | THR | 1223 | | -13.590 | 55.210 | 1.00 19.60 |
| ATOM | 8161 | OG1 | THR | 1223 | | -13.785 | 56.332 | 1.00 20.12 |
| ATOM | 8162 | | THR | 1223 | | -12.709 | 55.625 | 1.00 23.60 |
| ATOM | 8163 | С | THR | 1223 | | -15.900 | 54.524 | 1.00 16.85 |
| MOTA | 8164 | 0 | THR | 1223 | | -16.719 | 55.398 | 1.00 16.75 |
| ATOM | 8165 | N | ALA | 1224 | | -15.801 | 53.386 | 1.00 16.57 |
| ATOM | 8166 | CA | ALA | 1224 | | -16.643 | 53.098 | 1.00 16.77 |
| ATOM | 8167 | CB | ALA | 1224 | | -17.980 | 52.530 | 1.00 16.53 |
| ATOM | 8168 | С | ALA | 1224 | | -15.886 | 52.099 | 1.00 15.47 |
| ATOM | 8169 | 0 | ALA | 1224 | | -15.171 | 51.243 | 1.00 13.50 |
| MOTA | 8170 | N | TYR | 1225 | | -16.043 | 52.203 | 1.00 13.85 |
| ATOM | 8171 | CA | TYR | 1225 | | -15.321 | 51.318 | 1.00 14.02 |
| ATOM | 8172 | CB | TYR | 1225 | | -14.088 | 52.033 | 1.00 16.12 |
| MOTA | 8173 | CG | TYR | 1225 | | -13.344 | 52.918 | 1.00 16.49 |
| MOTA | 8174 | CD1 | | 1225 | | -13.577 | 54.293 | 1.00 17.47 |
| ATOM | 8175 | | TYR | 1225 | | -12.901 | 55.118 | 1.00 19.34 |
| ATOM | 8176 | CD2 | TYR | 1225 | | -12.411 | 52.382 | 1.00 16.05 |
| MOTA | 8177 | CE2 | TYR | 1225 | | -11.728 | 53.197 | 1.00 17.27 |
| ATOM | 8178 | CZ | TYR | 1225 | | -11.982 | 54.566 | 1.00 17.92 |
| ATOM | 8179 | OH | TYR | 1225 | | -11.324 | 55.374 | 1.00 18.55 |
| ATOM | 8180 | С | TYR | 1225 | | -16.158 | 50.807 | 1.00 15.21 |
| ATOM | 8181 | 0 | TYR | 1225 | | -15.630 | 50.183 | 1.00 16.68 |
| MOTA | 8182 | N | ASP | 1226 | | -17.458 | 51.071 | 1.00 14.35 |
| ATOM | 8183 | CA | ASP | 1226 | | -18.321 | 50.620 | 1.00 14.15 |
| ATOM | 8184 | CB | ASP | 1226 | | -18.262 | 51.615 | 1.00 12.62 |
| ATOM | 8185 | CG | ASP | 1226 | | -18.827 | 52.983 | 1.00 15.38 |
| ATOM | 8186 | OD1 | | 1226 | | -20.064 | 53.099 | 1.00 14.85 |
| MOTA | 8187 | OD2 | ASP | 1226 | | -18.025 | 53.933 | 1.00 15.68 |
| MOTA | 8188 | С | ASP | 1226 | | -19.749 | 50.435 | 1.00 14.71 |
| MOTA | 8189 | 0 | ASP | 1226 | | -20.113 | 50.864 | 1.00 13.48 |
| MOTA | 8190 | N | TYR | 1227 | 2.604 | -20.548 | 49.780 | 1.00 13.68 |

| ATOM | 8191 | CA | TYR | 1227 | 2.312 -21.94 | 49.490 | 1.00 12.77 |
|------|------|-----|-----|------|----------------|----------|------------|
| MOTA | 8192 | CB | TYR | 1227 | 3.454 -22.52 | | 1.00 13.53 |
| ATOM | 8193 | CG | TYR | 1227 | 3.407 -24.02 | | 1.00 14.63 |
| ATOM | 8194 | CD1 | | 1227 | 2.642 -24.61 | | 1.00 15.74 |
| | 8195 | CE1 | TYR | 1227 | 2.594 -25.99 | | 1.00 16.62 |
| ATOM | | CD2 | | | | | 1.00 17.93 |
| MOTA | 8196 | | TYR | 1227 | 4.128 -24.86 | | |
| MOTA | 8197 | CE2 | TYR | 1227 | 4.087 -26.25 | | 1.00 16.82 |
| ATOM | 8198 | cz | TYR | 1227 | 3.325 -26.80 | | 1.00 19.67 |
| MOTA | 8199 | ОН | TYR | 1227 | 3.296 -28.17 | | 1.00 20.34 |
| MOTA | 8200 | С | TYR | 1227 | 2.104 -22.82 | 50.721 | 1.00 14.61 |
| ATOM | 8201 | 0 | TYR | 1227 | 1.169 -23.63 | 50.770 | 1.00 13.84 |
| MOTA | 8202 | N | SER | 1228 | 2.985 -22.67 | 7 51.704 | 1.00 15.14 |
| ATOM | 8203 | CA | SER | 1228 | 2.932 -23.48 | 3 52.915 | 1.00 17.24 |
| MOTA | 8204 | CB | SER | 1228 | 4.115 -23.15 | 53.821 | 1.00 17.68 |
| MOTA | 8205 | OG | SER | 1228 | 5.330 -23.53 | | 1.00 20.49 |
| ATOM | 8206 | ď | SER | 1228 | 1.637 -23.40 | | 1.00 16.77 |
| ATOM | 8207 | õ | SER | 1228 | 1.012 -24.42 | | 1.00 17.76 |
| | 8208 | N | PHE | 1229 | 1.233 -22.19 | | 1.00 17.16 |
| MOTA | | | | | | | |
| MOTA | 8209 | CA | PHE | 1229 | -0.001 -22.05 | | 1.00 16.83 |
| MOTA | 8210 | CB | PHE | 1229 | -0.100 -20.66 | | 1.00 17.59 |
| ATOM | 8211 | CG | PHE | 1229 | 0.713 -20.52 | | 1.00 17.48 |
| MOTA | 8212 | CD1 | | 1229 | 1.969 -19.92 | | 1.00 19.55 |
| MOTA | 8213 | CD2 | PHE | 1229 | 0.239 -21.04 | 57.916 | 1.00 20.98 |
| MOTA | 8214 | CE1 | PHE | 1229 | 2.749 -19.85 | 57.844 | 1.00 19.23 |
| ATOM | 8215 | CE2 | PHE | 1229 | 1.009 -20.97 | 59.076 | 1.00 21.94 |
| ATOM | 8216 | CZ | PHE | 1229 | 2.267 -20.37 | 59.038 | 1.00 20.88 |
| ATOM | 8217 | C | PHE | 1229 | -1.226 -22.35 | | 1.00 16.51 |
| ATOM | 8218 | ō | PHE | 1229 | -2.190 -22.92 | | 1.00 16.61 |
| ATOM | 8219 | N | ALA | 1230 | -1.198 -21.97 | | 1.00 15.96 |
| ATOM | 8220 | CA | ALA | 1230 | -2.340 -22.24 | | 1.00 17.17 |
| | | | | | | | |
| MOTA | 8221 | СВ | ALA | 1230 | -2.103 -21.65 | | 1.00 15.08 |
| MOTA | 8222 | C | ALA | 1230 | -2.576 -23.75 | | 1.00 17.32 |
| MOTA | 8223 | 0 | ALA | 1230 | -3.715 -24.21 | | 1.00 18.17 |
| MOTA | 8224 | N | LYS | 1231 | -1.493 -24.51 | | 1.00 17.85 |
| MOTA | 8225 | CA | LYS | 1231 | -1.577 -25.97 | | 1.00 18.56 |
| MOTA | 8226 | CB | LYS | 1231 | -0.186 -26.54 | 51.201 | 1.00 19.63 |
| ATOM | 8227 | CG | LYS | 1231 | -0.100 -28.07 | 51.122 | 1.00 23.84 |
| MOTA | 8228 | CD | LYS | 1231 | -0.869 -28.63 | 49.940 | 1.00 29.01 |
| ATOM | 8229 | CE | LYS | 1231 | -0.484 -30.08 | 49.634 | 1.00 31.79 |
| ATOM | 8230 | NZ | LYS | 1231 | -0.862 -31.05 | | 1.00 35.95 |
| ATOM | 8231 | C | LYS | 1231 | -2.127 -26.56 | | 1.00 17.93 |
| ATOM | 8232 | ō | LYS | 1231 | -2.990 -27.44 | | 1.00 19.83 |
| | | N | | 1232 | -1.626 -26.07 | | 1.00 19.47 |
| MOTA | 8233 | | LEU | | | | |
| ATOM | | CA | LEU | 1232 | -2.063 -26.55 | | 1.00 18.49 |
| MOTA | 8235 | CB | LEU | 1232 | -1.265 -25.86 | | 1.00 20.15 |
| MOTA | 8236 | CG | LEU | 1232 | -1.474 -26.36 | | 1.00 20.23 |
| MOTA | 8237 | CD1 | LEU | 1232 | -0.235 -26.10 | | 1.00 20.74 |
| MOTA | 8238 | CD2 | LEU | 1232 | -2.691 -25.67 | 58.358 | 1.00 20.65 |
| MOTA | 8239 | C. | LEU | 1232 | -3.566 -26.31 | 55.394 | 1.00 19.99 |
| ATOM | 8240 | 0 | LEU | 1232 | -4.311 -27.22 | 55.777 | 1.00 19.78 |
| ATOM | 8241 | N | PHE | 1233 | -4.013 -25.10 | 55.095 | 1.00 18.10 |
| ATOM | 8242 | CA | | 1233 | -5.430 -24.77 | | 1.00 20.73 |
| ATOM | 8243 | CB | PHE | 1233 | -5.701 -23.30 | 54.844 | 1.00 18.29 |
| ATOM | 8244 | CG | PHE | 1233 | -4.957 -22.30 | | 1.00 18.77 |
| ATOM | 8245 | | PHE | 1233 | -4.606 -22.59 | | 1.00 18.49 |
| ATOM | 8246 | | PHE | 1233 | -4.628 -21.06 | | 1.00 18.49 |
| | | | | | | | 1.00 17.01 |
| ATOM | 8247 | | PHE | 1233 | -3.940 -21.65 | | |
| MOTA | 8248 | CE2 | | 1233 | -3.961 -20.11 | | 1.00 15.70 |
| MOTA | 8249 | CZ | PHE | 1233 | -3.618 -20.413 | | 1.00 17.50 |
| ATOM | 8250 | С | PHE | 1233 | -6.278 -25.67 | | 1.00 21.36 |
| MOTA | 8251 | 0 | PHE | 1233 | -7.299 -26.21 | | 1.00 22.69 |
| ATOM | 8252 | . N | ALA | 1234 | -5.859 -25.840 | | 1.00 21.60 |
| ATOM | 8253 | CA | ALA | 1234 | -6.601 -26.67 | 52.147 | 1.00 21.61 |
| MOTA | 8254 | CB | ALA | 1234 | -5.960 -26.61 | 50.758 | 1.00 21.86 |
| MOTA | 8255 | C | ALA | 1234 | -6.709 -28.13 | | 1.00 23.65 |
| ATOM | 8256 | ō | ALA | 1234 | -7.759 -28.75 | | 1.00 19.72 |
| ATOM | 8257 | N | ASP | 1235 | -5.634 -28.67 | | 1.00 23.15 |
| ATOM | 8258 | CA | ASP | 1235 | -5.674 -30.06 | | 1.00 25.15 |
| | | | | | -4.264 -30.57° | | 1.00 26.19 |
| ATOM | 8259 | CB | ASP | 1235 | | | |
| ATOM | 8260 | CG | ASP | 1235 | -3.330 -30.562 | | 1.00 30.30 |
| ATOM | 8261 | | ASP | 1235 | -3.758 -30.943 | | 1.00 29.31 |
| ATOM | 8262 | | ASP | 1235 | -2.153 -30.189 | | 1.00 30.67 |
| MOTA | 8263 | С | ASP | 1235 | -6.561 -30.210 | | 1.00 25.67 |
| MOTA | 8264 | 0 | ASP | 1235 | -6.896 -31.333 | | 1.00 27.41 |
| MOTA | 8265 | N | GLU | 1236 | -6.935 -29.09 | | 1.00 26.80 |
| ATOM | 8266 | CA | GLU | 1236 | -7.779 -29.13 | 56.693 | 1.00 28.17 |
| ATOM | 8267 | CB | GLU | 1236 | -7.236 -28.16 | | 1.00 28.31 |
| | | | | | | | |

| ATOM | 8268 | CG | GLU | 1236 | -5.900 | -28.583 | 58.322 | 1.00 30.31 |
|--------|--------------|-----|-----|------|---------|---------|--------|------------|
| ATOM | 8269 | CD | GLU | 1236 | | -29.977 | 58.913 | 1.00 30.97 |
| ATOM | 8270 | | GLU | 1236 | | -30.252 | 59.709 | 1.00 32.20 |
| ATOM | 8271 | OE2 | | 1236 | | -30.797 | 58.587 | 1.00 34.13 |
| | | | | | | -28.805 | 56.407 | 1.00 34.13 |
| ATOM | 8272 | C | GLU | 1236 | | | | |
| ATOM | 8273 | 0 | GLU | 1236 | | -28.956 | 57.277 | 1.00 29.70 |
| ATOM | 8274 | N | GLY | 1237 | | -28.348 | 55.194 | 1.00 28.96 |
| ATOM | 8275 | CA | GLY | 1237 | | -28.032 | 54.863 | 1.00 30.43 |
| MOTA | 8276 | С | GLY | 1237 | -11.165 | -26.570 | 54.567 | 1.00 29.93 |
| ATOM | 8277 | 0 | GLY | 1237 | -12.165 | -26.248 | 53.937 | 1.00 32.59 |
| MOTA | 8278 | N | LEU | 1238 | -10.286 | -25.684 | 55.033 | 1.00 28.83 |
| MOTA | 8279 | CA | LEU | 1238 | -10.449 | -24.257 | 54.771 | 1.00 28.65 |
| MOTA | 8280 | CB | LEU | 1238 | -9.434 | -23.438 | 55.568 | 1.00 28.60 |
| MOTA | 8281 | CG | LEU | 1238 | | -22.829 | 56.866 | 1.00 30.97 |
| ATOM | 8282 | | LEU | 1238 | | -22.052 | 57.548 | 1.00 29.17 |
| ATOM | 8283 | CD2 | | 1238 | | -21.918 | 56.559 | 1.00 30.61 |
| ATOM | 8284 | C | LEU | 1238 | | -24.039 | 53.283 | 1.00 26.94 |
| | | | | | -9.085 | | | 1.00 27.39 |
| MOTA | 8285 | 0 | LEU | 1238 | | | 52.835 | |
| ATOM | 8286 | N | ASN | 1239 | | -23.948 | 52.523 | 1.00 24.94 |
| MOTA | 8287 | CA | ASN | 1239 | | -23.782 | 51.080 | 1.00 24.45 |
| MOTA | 8288 | CB | ASN | 1239 | | -24.803 | 50.369 | 1.00 26.67 |
| ATOM | 8289 | CG | ASN | 1239 | | -26.213 | 50.844 | 1.00 29.98 |
| MOTA | 8290 | OD1 | ASN | 1239 | -10.690 | -26.664 | 50.903 | 1.00 31.35 |
| ATOM | 8291 | ND2 | ASN | 1239 | -12.905 | -26.924 | 51.188 | 1.00 33.26 |
| ATOM | 8292 | С | ASN | 1239 | -11.527 | -22.391 | 50.573 | 1.00 22.89 |
| ATOM | 8293 | 0 | ASN | 1239 | -11.763 | -22.201 | 49.382 | 1.00 24.50 |
| MOTA | 8294 | N | VAL | 1240 | -11.545 | -21.420 | 51.475 | 1.00 21.81 |
| ATOM | 8295 | CA | VAL | 1240 | | -20.039 | 51.086 | 1.00 19.80 |
| ATOM | 8296 | CB | VAL | 1240 | | -19.519 | 51.629 | 1.00 20.14 |
| ATOM | 8297 | | VAL | 1240 | | -18.098 | 51.141 | 1.00 18.87 |
| | | CG1 | | | | -20.413 | 51.176 | 1.00 10.07 |
| MOTA | 8298 | | | 1240 | | | | |
| MOTA | 8299 | C | VAL | 1240 | | -19.190 | 51.663 | 1.00 19.46 |
| MOTA | 8300 | Ó | VAL | 1240 | | -18.960 | 52.868 | 1.00 18.98 |
| ATOM | 8301 | N | MET | 1241 | | -18.719 | 50.788 | 1.00 18.30 |
| ATOM | 8302 | CA | MET | 1241 | | -17.922 | 51.210 | 1.00 17.27 |
| ATOM | 8303 | CB | MET | 1241 | -7.382 | -18.672 | 50.927 | 1.00 17.64 |
| MOTA | 8304 | CG | MET | 1241 | -7.204 | -19.922 | 51.769 | 1.00 18.74 |
| ATOM . | 8305 | SD | MET | 1241 | -5.840 | -20.926 | 51.216 | 1.00 19.35 |
| MOTA | 8306 | CE | MET | 1241 | -6.619 | -22.510 | 51.062 | 1.00 19.09 |
| ATOM | 8307 | C | MET | 1241 | | -16.583 | 50.521 | 1.00 16.92 |
| ATOM | 8308 | ō | MET | 1241 | | -16.469 | 49.348 | 1.00 17.62 |
| ATOM | 8309 | N | LEU | 1242 | | -15.571 | 51.249 | 1.00 16.36 |
| ATOM | 8310 | CA | LEU | 1242 | | -14.233 | 50.694 | 1.00 17.87 |
| | 8311 | | LEU | 1242 | | -13.270 | | 1.00 17.87 |
| ATOM | | CB | | | | | 51.501 | |
| ATOM | 8312 | CG | LEU | 1242 | | -11.757 | 51.253 | 1.00 23.91 |
| ATOM | 8313 | CD1 | | 1242 | | -11.072 | 51.987 | 1.00 25.91 |
| MOTA | 8314 | CD2 | | 1242 | | -11.402 | 49.770 | 1.00 21.85 |
| MOTA | 8315 | С | LEU | 1242 | -6.625 | -13.759 | 50.682 | 1.00 16.01 |
| MOTA | 8316 | O | LEU | 1242 | -5.911 | -13.860 | 51.679 | 1.00 14.63 |
| ATOM | 8317 | N | VAL | 1243 | -6.202 | -13.259 | 49.529 | 1.00 16.58 |
| ATOM | 8318 | CA | VAL | 1243 | -4.859 | -12.724 | 49.381 | 1.00 15.62 |
| ATOM | 8319 | CB | VAL | 1243 | -4.233 | -13.152 | 48.046 | 1.00 15.84 |
| ATOM | 8320 | CG1 | VAL | 1243 | -2.801 | -12.644 | 47.954 | 1.00 15.84 |
| ATOM | 8321 | | VAL | 1243 | | -14.668 | 47.923 | 1.00 17.35 |
| ATOM | 8322 | C | VAL | 1243 | | -11.223 | 49.413 | 1.00 15.28 |
| ATOM | 8323 | o | VAL | 1243 | -5.272 | | 48.376 | 1.00 14.94 |
| ATOM | 8324 | N | GLY | 1244 | | -10.662 | 50.622 | 1.00 16.14 |
| | | | , | | -5.351 | | 50.622 | 1.00 18.14 |
| ATOM | 8325 | CA | GLY | 1244 | | -9.244 | | |
| ATOM | 8326 | C | GLY | 1244 | -4.156 | -8.347 | 50.980 | 1.00 16.28 |
| ATOM | 8327 | 0 | GLY | 1244 | -3.061 | -8.815 | 51.306 | 1.00 14.05 |
| MOTA | 8328 | N | ASP | 1245 | -4.368 | -7.046 | 50.798 | 1.00 17.20 |
| MOTA | 832 9 | CA | ASP | 1245 | -3.276 | -6.105 | 50.957 | 1.00 17.71 |
| MOTA | 8330 | CB | ASP | 1245 | -3.620 | -4.728 | 50.369 | 1.00 17.04 |
| ATOM | 8331 | CG | ASP | 1245 | -4.889 | -4.121 | 50.952 | 1.00 16.86 |
| ATOM | 8332 | OD1 | ASP | 1245 | -5.415 | -4.640 | 51.951 | 1.00 16.51 |
| ATOM | 8333 | | ASP | 1245 | -5.338 | -3.111 | 50.384 | 1.00 17.00 |
| MOTA | 8334 | С | ASP | 1245 | -2.837 | -5.978 | 52.404 | 1.00 16.69 |
| ATOM | 8335 | Õ | ASP | 1245 | -1.944 | -5.202 | 52.715 | 1.00 15.57 |
| ATOM | 8336 | N | SER | 1246 | -3.471 | -6.736 | 53.291 | 1.00 16.51 |
| ATOM | 8337 | | | 1246 | -3.050 | -6.722 | 54.685 | 1.00 18.08 |
| | | CA | SER | | -3.963 | -7.606 | 55.539 | 1.00 13.08 |
| ATOM | 8338 | CB | SER | 1246 | | | | |
| ATOM | 8339 | OG | SER | 1246 | -4.087 | -8.920 | 55.004 | 1.00 20.35 |
| ATOM | 8340 | C | SER | 1246 | -1.617 | -7.262 | 54.687 | 1.00 17.95 |
| ATOM | 8341 | 0 | SER | 1246 | -0.865 | -7.062 | 55.642 | 1.00 18.43 |
| ATOM | 8342 | N | LEU | 1247 | -1.234 | -7.943 | 53.606 | 1.00 17.78 |
| ATOM | 8343 | CA | LEU | 1247 | 0.131 | -8.473 | 53.503 | 1.00 17.35 |
| MOTA | 8344 | CB | LEU | 1247 | 0.302 | -9.318 | 52.225 | 1.00 16.63 |
| | | | | | | | | |

| ATOM | 8345 | CG | LEU | 1247 | 0.200 | -8.648 | 50.854 | 1.00 14.50 |
|------|-------|-----|-------|------|--------|---------|--------|------------|
| ATOM | 8346 | CD1 | LEU | 1247 | 1.513 | -7.956 | 50.524 | 1.00 14.50 |
| ATOM | 8347 | CD2 | | 1247 | -0.135 | -9.688 | 49.777 | 1.00 14.80 |
| ATOM | 8348 | c | LEU | 1247 | 1.143 | -7.323 | 53.521 | 1.00 15.79 |
| ATOM | 8349 | ō | LEU | 1247 | 2.330 | -7.520 | 53.796 | 1.00 14.98 |
| ATOM | 8350 | N | GLY | 1248 | 0.682 | -6.116 | 53.730 | 1.00 13.56 |
| | | | | | | - | | 1.00 13.36 |
| ATOM | 8351 | CA | GLY | 1248 | 1.584 | -4.978 | 53.226 | |
| MOTA | 8352 | С | GLY | 1248 | 2.119 | -4.763 | 54.624 | 1.00 15.47 |
| ATOM | 8353 | 0 | GLY | 1248 | 3.228 | -4.261 | 54.820 | 1.00 16.88 |
| MOTA | 8354 | N | MET | 1249 | 1.325 | -5.162 | 55.608 | 1.00 14.33 |
| MOTA | 8355 | CA | MET | 1249 | 1.719 | -5.005 | 56.996 | 1.00 16.01 |
| MOTA | 8356 | CB | MET | 1249 | 0.513 | -4.502 | 57.800 | 1.00 19.46 |
| ATOM | 8357 | CG | MET | 1249 | 0.018 | -3.144 | 57.322 | 1.00 21.69 |
| MOTA | 8358 | SD | MET | 1249 | -1.516 | -2.566 | 58.097 | 1.00 26.00 |
| MOTA | 8359 | CE | MET | 1249 | -0.965 | -2.281 | 59.756 | 1.00 27.35 |
| ATOM | 8360 | C | MET | 1249 | 2.290 | -6.289 | 57.602 | 1.00 16.59 |
| ATOM | 8361 | ,0 | MET | 1249 | 3.417 | -6.305 | 58.096 | 1.00 14.81 |
| | 8362 | N | THR | 1250 | 1.525 | -7.369 | 57.530 | 1.00 16.12 |
| ATOM | | | | | | | | |
| ATOM | 8363 | CA | THR | 1250 | 1.946 | -8.636 | 58.100 | 1.00 18.02 |
| ATOM | 8364 | CB | THR | 1250 | 0.751 | -9.598 | 58.167 | 1.00 19.93 |
| ATOM | 8365 | OG1 | | 1250 | 1.098 | -10.759 | 58.930 | 1.00 25.56 |
| ATOM | 8366 | CG2 | THR | 1250 | 0.341 | -10.019 | 56.777 | 1.00 21.14 |
| ATOM | 8367 | С | THR | 1250 | 3.111 | -9.311 | 57.368 | 1.00 16.42 |
| ATOM | 8368 | 0 | THR | 1250 | 3.920 | -10.011 | 57.982 | 1.00 17.25 |
| ATOM | 8369 | N | VAL | 1251 | 3.207 | -9.114 | 56.060 | 1.00 14.38 |
| ATOM | 8370 | CA | VAL | 1251 | 4.295 | -9.729 | 55.306 | 1.00 14.53 |
| ATOM | 8371 | СВ | VAL | 1251 | 3.792 | -10.309 | 53.953 | 1.00 15.45 |
| ATOM | 8372 | | VAL | 1251 | 4.975 | -10.833 | 53.133 | 1.00 12.75 |
| ATOM | 8373 | CG2 | | 1251 | 2.796 | -11.428 | 54.210 | 1.00 15.08 |
| ATOM | 8374 | C | VAL | 1251 | 5.419 | -8.732 | 55.039 | 1.00 14.56 |
| | | | | | 6.573 | -8.978 | | |
| ATOM | 8375 | 0 | VAL | 1251 | | | 55.395 | 1.00 16.60 |
| MOTA | 8376 | N | GLN | 1252 | 5.077 | -7.598 | 54.437 | 1.00 11.43 |
| MOTA | 8377 | CA | GLN | 1252 | 6.064 | -6.574 | 54.097 | 1.00 13.81 |
| ATOM | 8378 | CB | GLN | 1252 | 5.493 | -5.649 | 53.026 | 1.00 14.06 |
| MOTA | 8379 | CG | GLN | 1252 | 4.925 | -6.404 | 51.832 | 1.00 15.86 |
| MOTA | 8380 | CD | GLN | 1252 | 4.458 | -5.482 | 50.727 | 1.00 14.76 |
| MOTA | 8381 | OE1 | GLN | 1252 | 4.178 | -4.304 | 50.960 | 1.00 14.09 |
| ATOM | 8382 | NE2 | GLN | 1252 | 4.358 | -6.019 | 49.513 | 1.00 12.71 |
| ATOM | 8383 | C | GLN | 1252 | 6.581 | -5.742 | 55.270 | 1.00 14.83 |
| ATOM | 8384 | 0 | GLN | 1252 | 7.726 | -5.291 | 55.249 | 1.00 15.58 |
| MOTA | 8385 | N | GLY | 1253 | 5.739 | -5.523 | 56.272 | 1.00 15.09 |
| ATOM | 8386 | CA | GLY | 1253 | 6.165 | -4.760 | 57.434 | 1.00 15.66 |
| | 8387 | C | GLY | 1253 | 5.888 | -3.269 | 57.397 | 1.00 17.26 |
| ATOM | | | | | | | | |
| ATOM | 8388 | 0 | GLY | 1253 | 6.480 | -2.501 | 58.163 | 1.00 18.18 |
| ATOM | 8389 | N | HIS | 1254 | 5.001 | -2.838 | 56.509 | 1.00 17.51 |
| ATOM | 8390 | CA | HIS | 1254 | 4.671 | -1.420 | 56.429 | 1.00 18.70 |
| ATOM | 8391 | CB | HIS | 1254 | 4.126 | -1.065 | 55.045 | 1.00 19.45 |
| MOTA | 8392 | CG | HIS | 1254 | 5.119 | -1.251 | 53.945 | 1.00 19.97 |
| MOTA | 8393 | CD2 | HIS | 1254 | 5.122 | -2.083 | 52.876 | 1.00 19.30 |
| MOTA | 8394 | ND1 | HIS | 1254 | 6.287 | -0.522 | 53.868 | 1.00 18.30 |
| MOTA | 8395 | CE1 | HIS | 1254 | 6.965 | -0.896 | 52.798 | 1.00 22.21 |
| ATOM | 8396 | | HIS | 1254 | 6.280 | -1.841 | 52.178 | 1.00 21.62 |
| ATOM | 8397 | C | HIS | 1254 | 3.634 | -1.094 | 57.488 | 1.00 18.59 |
| ATOM | 8398 | ō | HIS | 1254 | 2.986 | -1.996 | 58.025 | 1.00 19.51 |
| ATOM | 8399 | N | ASP | 1255 | 3.487 | 0.192 | 57.788 | 1.00 19.71 |
| ATOM | 8400 | CA | ASP | 1255 | 2.530 | 0.651 | 58.795 | 1.00 23.34 |
| | | | | | | 2.030 | 59.331 | 1.00 27.63 |
| MOTA | 8401 | CB | ASP | 1255 | 2.943 | | | |
| ATOM | 8402 | CG | ASP | 1255 | 3.048 | 3.077 | 58.239 | 1.00 29.81 |
| MOTA | 8403 | | ASP | 1255 | 2.101 | 3.214 | 57.443 | 1.00 33.96 |
| MOTA | 8404 | | ASP | 1255 | 4.082 | 3.776 | 58.178 | 1.00 37.20 |
| MOTA | 8405 | С | ASP | 1255 | 1.096 | 0.712 | 58.272 | 1.00 21.29 |
| MOTA | 8406 | 0 | ASP | 1255 | 0.156 | 0.883 | 59.047 | 1.00 21.48 |
| MOTA | 8407 | N | SER | 1256 | 0.931 | 0.587 | 56.958 | 1.00 19.07 |
| MOTA | 8408 | CA | SER | 1256 | -0.398 | 0.609 | 56.339 | 1.00 16.19 |
| MOTA | 8409 | CB | SER | 1256 | -0.761 | 2.024 | 55.869 | 1.00 14.13 |
| ATOM | 8410 | OG | SER | 1256 | 0.016 | 2.418 | 54.748 | 1.00 13.20 |
| ATOM | 8411 | C | SER | 1256 | -0.394 | -0.339 | 55.141 | 1.00 16.00 |
| ATOM | 8412 | ō | SER | 1256 | 0.628 | -0.956 | 54.838 | 1.00 16.64 |
| ATOM | 8413 | N | THR | 1257 | -1.526 | -0.444 | 54.453 | 1.00 15.54 |
| | | | | | -1.616 | -1.327 | 53.296 | 1.00 13.34 |
| ATOM | 8414 | CA | THR | 1257 | | | | |
| ATOM | 8415 | CB | THR | 1257 | -3.001 | -2.009 | 53.214 | 1.00 14.68 |
| ATOM | .8416 | | THR | 1257 | -4.005 | -1.020 | 52.942 | 1.00 13.16 |
| ATOM | 8417 | CG2 | THR | 1257 | -3.333 | -2.708 | 54.518 | 1.00 14.28 |
| ATOM | 8418 | С | THR | 1257 | -1.383 | -0.596 | 51.978 | 1.00 14.73 |
| MOTA | 8419 | 0 | THR | 1257 | -1.260 | -1.232 | 50.931 | 1.00 14.37 |
| ATOM | 8420 | N | LEU | 1258 | -1.296 | 0.731 | 52.028 | 1.00 11.56 |
| | | ~~ | LEU | 1258 | -1.116 | 1.522 | 50.810 | 1.00 14.62 |
| ATOM | 8421 | CA | LIE C | 1250 | | | | |

| ATOM | 8422 | CB | LEU | 1258 | -1.059 | 3.022 | 51.151 | 1.00 14.76 |
|---------|------|-----|------|------|--------|---------|--------|------------|
| | | | | | | | | |
| MOTA | 8423 | CG | LEU | 1258 | -2.415 | 3.708 | 51.387 | 1.00 18.81 |
| ATOM | 8424 | CD1 | LEU | 1258 | -3.037 | 3.193 | 52.689 | 1.00 18.31 |
| ATOM | 8425 | CD2 | LEU | 1258 | -2.225 | 5.211 | 51.451 | 1.00 17.89 |
| ATOM | 8426 | С | LEU | 1258 | 0.049 | 1.172 | 49.873 | 1.00 13.86 |
| | | | | | | | | |
| MOTA | 8427 | 0 | LEU | 1258 | -0.099 | 1.248 | 48.655 | 1.00 13.08 |
| ATOM | 8428 | N | PRO | 1259 | 1.215 | 0.790 | 50.419 | 1.00 15.27 |
| ATOM | 8429 | CD | PRO | 1259 | 1.610 | 0.817 | 51.836 | 1.00 16.92 |
| | | | PRO | 1259 | 2.355 | 0.448 | 49.562 | 1.00 13.94 |
| MOTA | 8430 | CA | | | | | | |
| ATOM | 8431 | CB | PRO | 1259 | 3.521 | 0.372 | 50.544 | 1.00 17.82 |
| ATOM | 8432 | CG | PRO | 1259 | 2.850 | -0.036 | 51.830 | 1.00 22.73 |
| ATOM | 8433 | С | PRO | 1259 | 2.208 | -0.827 | 48.733 | 1.00 13.69 |
| | | | | | | | | 1.00 11.25 |
| ATOM | 8434 | 0 | PRO | 1259 | 2.956 | -1.020 | 47.779 | |
| ATOM | 8435 | N | VAL | 1260 | 1.254 | -1.689 | 49.081 | 1.00 12.02 |
| MOTA | 8436 | CA | VAL | 1260 | 1.061 | -2.932 | 48.330 | 1.00 12.65 |
| ATOM | 8437 | CB | VAL | 1260 | -0.025 | -3.825 | 48.981 | 1.00 12.45 |
| | | | | | | | | |
| ATOM | 8438 | | VAL | 1260 | -0.258 | -5.057 | 48.132 | 1.00 11.57 |
| MOTA | 8439 | CG2 | VAL | 1260 | 0.401 | -4.235 | 50.391 | 1.00 9.00 |
| MOTA | 8440 | С | VAL | 1260 | 0.659 | -2.631 | 46.892 | 1.00 12.91 |
| | | | VAL | | -0.252 | -1.834 | 46.638 | 1.00 12.38 |
| MOTA | 8441 | 0 | | 1260 | | | | |
| MOTA | 8442 | N | THR | 1261 | 1.325 | -3.281 | 45.941 | 1.00 14.02 |
| ATOM | 8443 | CA | THR | 1261 | 1.019 | -3.060 | 44.529 | 1.00 13.63 |
| ATOM | 8444 | CB | THR | 1261 | 2.326 | -2.816 | 43.724 | 1.00 18.67 |
| | | | | 1261 | | -1.749 | | 1.00 18.95 |
| MOTA | 8445 | OG1 | THR | | 3.072 | | 44.337 | |
| MOTA | 8446 | CG2 | THR | 1261 | 2.010 | -2.410 | 42.285 | 1.00 22.02 |
| MOTA | 8447 | С | THR | 1261 | 0.268 | -4.259 | 43.930 | 1.00 12.64 |
| ATOM | 8448 | Ō | THR | 1261 | 0.115 | -5.289 | 44.572 | 1.00 11.51 |
| | | | | | | | | |
| ATOM | 8449 | N | VAL | 1262 | -0.197 | -4.108 | 42.697 | 1.00 10.72 |
| ATOM | 8450 | CA | VAL | 1262 | -0.906 | -5.181 | 42.017 | 1.00 11.46 |
| MOTA | 8451 | CB | VAL | 1262 | -1.484 | -4.682 | 40.675 | 1.00 10.61 |
| | | | | | -2.069 | | 39.875 | 1.00 10.47 |
| MOTA | 8452 | CG1 | VAL | 1262 | | -5.852 | | |
| MOTA | 8453 | CG2 | VAL | 1262 | -2.576 | -3.631 | 40.956 | 1.00 10.70 |
| ATOM | 8454 | C | VAL | 1262 | 0.068 | -6.339 | 41.790 | 1.00 11.29 |
| MOTA | 8455 | 0 | VAL | 1262 | -0.310 | -7.511 | 41.895 | 1.00 11.57 |
| | | | | | | | | |
| MOTA | 8456 | N | ALA | 1263 | 1.324 | -6.006 | 41.497 | 1.00 12.19 |
| MOTA | 8457 | CA | ALA | 1263 | 2.339 | -7.031 | 41.275 | 1.00 11.44 |
| MOTA | 8458 | CB | ALA | 1263 | 3.673 | -6.389 | 40.842 | 1.00 11.79 |
| ATOM | 8459 | C | ALA | 1263 | 2.531 | -7.843 | 42.556 | 1.00 11.93 |
| | | | | | | | | |
| MOTA | 8460 | 0 | ALA | 1263 | 2.724 | -9.065 | 42.505 | 1.00 10.47 |
| ATOM | 8461 | N | ASP | 1264 | 2.491 | -7.172 | 43.708 | 1.00 9.71 |
| ATOM | 8462 | CA | ASP | 1264 | 2.648 | -7.883 | 44.981 | 1.00 13.19 |
| ATOM | 8463 | CB | ASP | 1264 | 2.646 | -6.916 | 46.177 | 1.00 12.97 |
| | | | | | | | | |
| ATOM | 8464 | CG | ASP | 1264 | 3.782 | -5.904 | 46.135 | 1.00 15.35 |
| MOTA | 8465 | OD1 | ASP | 1264 | 4.833 | -6.206 | 45.548 | 1.00 13.99 |
| MOTA | 8466 | | ASP | 1264 | 3.635 | -4.805 | 46.713 | 1.00 12.70 |
| | 8467 | C | ASP | 1264 | 1.498 | -8.873 | 45.157 | 1.00 11.29 |
| MOTA | | | | | | | | |
| ATOM | 8468 | 0 | ASP | 1264 | | -10.036 | 45.488 | 1.00 12.23 |
| ATOM | 8469 | N | ILE | 1265 | 0.279 | -8.406 | 44.920 | 1.00 10.36 |
| ATOM | 8470 | CA | ILE | 1265 | -0.886 | -9.263 | 45.053 | 1.00 9.25 |
| | | | | | -2.194 | -8.492 | 44.733 | 1.00 8.35 |
| ATOM | 8471 | СВ | ILE | 1265 | | | | |
| ATOM | 8472 | CG2 | ILE | 1265 | -3.381 | -9.460 | 44.721 | 1.00 10.20 |
| ATOM | 8473 | CG1 | ILE | 1265 | -2.436 | -7.394 | 45.763 | 1.00 10.86 |
| ATOM | 8474 | CD1 | ILE | 1265 | -2.621 | -7.897 | 47.180 | 1.00 13.04 |
| | | | ILE | | | -10.474 | 44.125 | 1.00 10.11 |
| ATOM | 8475 | С | | 1265 | | | | |
| MOTA | 8476 | 0 | IĻE | 1265 | | -11.591 | 44.539 | 1.00 10.76 |
| MOTA | 8477 | N | ALA | 1266 | -0.373 | -10.259 | 42.878 | 1.00 11.37 |
| ATOM | 8478 | CA | ALA | 1266 | -0.269 | -11.361 | 41.915 | 1.00 10.83 |
| | | | ALA | 1266 | | -10.804 | 40.512 | 1.00 10.92 |
| ATOM | 8479 | CB | | | | | | |
| ATOM | 8480 | С | ALA | 1266 | | -12.398 | 42.299 | 1.00 10.56 |
| ATOM | 8481 | 0 | ALA | 1266 | 0.655 | -13.606 | 42.048 | 1.00 10.01 |
| ATOM | 8482 | N | TYR | 1267 | 1.882 | -11.919 | 42.905 | 1.00 9.93 |
| ATOM | 8483 | CA | TYR | 1267 | | -12.783 | 43.360 | 1.00 8.50 |
| | | | | | | | | |
| MOTA | 8484 | CB | TYR | 1267 | | -11.912 | 43.911 | 1.00 9.28 |
| ATOM | 8485 | CG | TYR | 1267 | 5.236 | -12.676 | 44.598 | 1.00 9.52 |
| ATOM | 8486 | CD1 | TYR | 1267 | 6.098 | -13.493 | 43.879 | 1.00 11.95 |
| ATOM | 8487 | CE1 | TYR | 1267 | | -14.176 | 44.509 | 1.00 12.07 |
| | | | | | | | | |
| ATOM | 8488 | CD2 | TYR | 1267 | | -12.559 | 45.972 | 1.00 12.37 |
| ATOM | 8489 | CE2 | TYR | 1267 | 6.475 | -13.237 | 46.615 | 1.00 12.84 |
| ATOM | 8490 | CZ | TYR | 1267 | 7.321 | -14.039 | 45.875 | 1.00 14.28 |
| | | | | | | -14.691 | 46.510 | 1.00 13.09 |
| ATOM | 8491 | OH | TYR | 1267 | | | | |
| ATOM | 8492 | С | TYR | 1267 | | -13.732 | 44.441 | 1.00 9.24 |
| ATOM | 8493 | 0 | TYR | 1267 | 2.636 | -14.960 | 44.368 | 1.00 7.23 |
| ATOM | 8494 | N | HIS | 1268 | | -13.162 | 45.448 | 1.00 10.07 |
| | | | | | | | | 1.00 11.40 |
| ATOM | 8495 | CA | HIS | 1268 | | -13.968 | 46.549 | |
| MOTA | 8496 | CB | HIS | 1268 | | -13.042 | 47.717 | 1.00 10.91 |
| MOTA | 8497 | CG | HIS | 1268 | 2.093 | -12.471 | 48.425 | 1.00 10.67 |
| ATOM | 8498 | | HIS | 1268 | | -11.277 | 48.299 | 1.00 12.54 |
| Y 1 OIJ | 0470 | CD2 | 1112 | 1200 | 2.120 | 11.4// | 30.433 | 2.00 IZ.JT |
| | | | | | | | | |

| MOTA | 8499 | ND1 | HIS | 1268 | 2.850 | -13.207 | 49.310 | 1.00 9.83 |
|------|-------|-----|------|------|-----------------------|---------|--------|------------|
| ATOM | 8500 | | HIS | 1268 | 3.896 | -12.495 | 49.694 | 1.00 12.36 |
| ATOM | 8501 | | HIS | 1268 | | -11.321 | 49.095 | 1.00 11.55 |
| | | | | | | -14.836 | 46.096 | 1.00 12.08 |
| MOTA | 8502 | C. | HIS | 1268 | | | | |
| MOTA | 8503 | 0 | HIS | 1268 | -0.104 | -15.933 | 46.610 | 1.00 10.75 |
| MOTA | 8504 | N | THR | 1269 | -0.655 | -14.351 | 45.112 | 1.00 11.50 |
| MOTA | 8505 | CA | THR | 1269 | -1.794 | -15.094 | 44.591 | 1.00 11.48 |
| ATOM | 85.06 | СВ | THR | 1269 | | -14.224 | 43.602 | 1.00 11.59 |
| ATOM | 8507 | OG1 | | 1269 | | -13.149 | 44.319 | 1.00 12.48 |
| | | | | | | | | |
| MOTA | 8508 | CG2 | THR | 1269 | | -15.039 | 42.884 | 1.00 13.07 |
| MOTA | 8509 | С | THR | 1269 | | -16.386 | 43.909 | 1.00 10.67 |
| MOTA | 8510 | 0 | THR | 1269 | -1.928 | -17.443 | 44.119 | 1.00 13.58 |
| ATOM | 8511 | N | ALA | 1270 | -0.292 | -16.301 | 43.098 | 1.00 8.94 |
| ATOM | 8512 | CA | ALA | 1270 | 0.228 | -17.478 | 42.414 | 1.00 10.29 |
| ATOM | 8513 | CB | ALA | 1270 | | -17.076 | 41.465 | 1.00 11.72 |
| | 8514 | C | ALA | 1270 | | -18.492 | 43.437 | 1.00 10.90 |
| ATOM | | | | | | | | |
| MOTA | 8515 | 0 | ALA | 1270 | | -19.701 | 43.269 | 1.00 12.02 |
| ATOM | 8516 | N | ALA | 1271 | | -17.998 | 44.495 | 1.00 11.07 |
| ATOM | 8517 | CA | ALA | 1271 | 1.924 | -18.878 | 45.534 | 1.00 11.19 |
| ATOM | 8518 | CB | ALA | 1271 | 2.733 | -18.064 | 46.541 | 1.00 10.42 |
| ATOM | 8519 | С | ALA | 1271 | 0.816 | -19.642 | 46.251 | 1.00 11.93 |
| ATOM | 8520 | ō | ALA | 1271 | | -20.849 | 46.458 | 1.00 9.16 |
| | | | | | | -18.922 | 46.645 | 1.00 12.77 |
| ATOM | 8521 | N | VAL | 1272 | | | | |
| ATOM | 8522 | CA | VAL | 1272 | | -19.528 | 47.331 | 1.00 12.55 |
| MOTA | 8523 | CB | VAL | 1272 | | -18.436 | 47.812 | 1.00 10.99 |
| ATOM | 8524 | CG1 | VAL | 1272 | -3.613 | -19.062 | 48.365 | 1.00 13.11 |
| MOTA | 8525 | CG2 | VAL | 1272 | -1.660 | -17.597 | 48.893 | 1.00 10.80 |
| ATOM | 8526 | С | VAL | 1272 | -2.063 | -20.535 | 46.436 | 1.00 12.93 |
| ATOM | 8527 | ō | VAL | 1272 | | -21.624 | 46.882 | 1.00 13.02 |
| | | | | | | -20.191 | | |
| MOTA | 8528 | | ARG | 1273 | | | 45.163 | |
| MOTA | 8529 | CA | ARG | 1273 | | -21.109 | 44.236 | 1.00 13.02 |
| ATOM | 8530 | CB | ARG | 1273 | -3.058 | -20.457 | 42.862 | 1.00 13.85 |
| ATOM | 8531 | CG | ARG | 1273 | -3.681 | -21.381 | 41.817 | 1.00 15.25 |
| ATOM | 8532 | ĊD | ARG | 1273 | -5.033 | -21.909 | 42.266 | 1.00 15.44 |
| ATOM | 8533 | NE | ARG | 1273 | | -20.917 | 42.171 | 1.00 15.46 |
| ATOM | 8534 | CZ | ARG | 1273 | | | 42.742 | 1.00 16.08 |
| | | | | | | | | |
| ATOM | 8535 | | ARG | 1273 | and the second second | -22.151 | 43.454 | 1.00 14.02 |
| MOTA | 8536 | | ARG | 1273 | | -20.120 | 42.592 | 1.00 14.57 |
| ATOM | 8537 | С | ARG | 1273 | | -22.410 | 44.088 | 1.00 14.78 |
| MOTA | 8538 | 0 | ARG | 1273 | -2.710 | -23.466 | 43.933 | 1.00 15.68 |
| MOTA | 8539 | N | ARG | 1274 | -0.777 | -22.337 | 44.123 | 1.00 13.54 |
| MOTA | 8540 | CA | ARG | 1274 | | -23.542 | 44.003 | 1.00 15.46 |
| ATOM | 8541 | СВ | ARG | 1274 | | -23.195 | 43.949 | 1.00 14.07 |
| | | | | | | | | |
| ATOM | 8542 | CG | ARG | 1274 | | -22.395 | 42.728 | 1.00 17.35 |
| ATOM | 8543 | CD | ARG | 1274 | | -22.383 | 42.532 | 1.00 16.78 |
| MOTA | 8544 | NE | ARG | 1274 | | -21.497 | 41.436 | 1.00 20.34 |
| ATOM | 8545 | CZ | ARG | 1274 | 4.066 | -20.203 | 41.573 | 1.00 20.54 |
| ATOM | 8546 | NH1 | ARG | 1274 | 4.038 | -19.634 | 42.772 | 1.00 Ì8.45 |
| MOTA | 8547 | NH2 | | 1274 | | -19.468 | 40.502 | 1.00 22.65 |
| ATOM | 8548 | С | ARG | 1274 | -0.222 | -24.468 | 45.185 | 1.00 16.23 |
| | | | | | | | 45.043 | 1.00 16.23 |
| MOTA | 8549 | 0 | ,ARG | 1274 | | -25.693 | | |
| MOTA | 8550 | N | GLY | 1275 | | -23.872 | 46.353 | 1.00 15.34 |
| ATOM | 8551 | CA | GLY | 1275 | -0.671 | -24.654 | 47.554 | 1.00 16.35 |
| MOTA | 8552 | С | GLY | 1275 | -2.105 | -25.138 | 47.686 | 1.00 17.09 |
| ATOM | 8553 | 0 | GLY | 1275 | -2.363 | -26.148 | 48.338 | 1.00 17.88 |
| MOTA | 8554 | N | ALA | 1276 | -3.042 | -24.417 | 47.077 | 1.00 15.42 |
| ATOM | 8555 | CA | ALA | 1276 | | -24.785 | 47.141 | 1.00 15.88 |
| ATOM | 8556 | CB | ALA | 1276 | | -23.921 | 48.170 | 1.00 12.41 |
| | | | | | | | | |
| ATOM | 8557 | С | ALA | 1276 | | -24.623 | 45.770 | 1.00 18.03 |
| ATOM | 8558 | 0 | ALA | 1276 | | -23.690 | 45.546 | 1.00 17.23 |
| MOTA | 8559 | N | PRO | 1277 | -4.843 | -25.550 | 44.841 | 1.00 19.05 |
| MOTA | 8560 | CD | PRO | 1277 | -4.009 | -26.751 | 45.029 | 1.00 21.91 |
| MOTA | 8561 | CA | PRO | 1277 | -5.402 | -25.507 | 43.486 | 1.00 20.89 |
| MOTA | 8562 | CB | PRO | 1277 | | -26.665 | 42.784 | 1.00 21.37 |
| ATOM | 8563 | CG | PRO | 1277 | | -27.631 | 43.890 | 1.00 23.97 |
| | | | | | | -25.574 | | |
| MOTA | 8564 | C | PRO | 1277 | | | 43.340 | 1.00 21.51 |
| ATOM | 8565 | 0 | PRO | 1277 | | -25.173 | 42.306 | 1.00 21.21 |
| MOTA | 8566 | N | ASN | 1278 | | -26.049 | 44.371 | 1.00 20.14 |
| MOTA | 8567 | CA | ASN | 1278 | -9.065 | -26.171 | 44.297 | 1.00 21.69 |
| MOTA | 8568 | CB | ASN | 1278 | -9.483 | -27.622 | 44.567 | 1.00 25.95 |
| MOTA | 8569 | CG | ASN | 1278 | -8.833 | -28.600 | 43.610 | 1.00 26.75 |
| ATOM | 8570 | OD1 | ASN | 1278 | -8.927 | -28.446 | 42.393 | 1.00 30.57 |
| | | | | | -8.173 | -29.612 | 44.154 | 1.00 30.37 |
| ATOM | 8571 | ND2 | | 1278 | | | | |
| MOTA | 8572 | С | ASN | 1278 | -9.823 | -25.245 | 45.235 | 1.00 21.44 |
| MOTA | 8573 | 0 | ASN | 1278 | -11.042 | | 45.364 | 1.00 20.63 |
| MOTA | 8574 | N | CYS | 1279 | -9.112 | -24.332 | 45.884 | 1.00 19.87 |
| MOTA | 8575 | CA | CYS | 1279 | -9.763 | -23.408 | 46.804 | 1.00 19.78 |
| | | | | | | | | |

| ATOM | 8576 | CB | CYS | 1279 | -8.749 | -22.831 | 47.799 | 1.00 19.93 | |
|------|------|-----|-----|------|---------|----------|--------|------------|---|
| | 8577 | SG | CYS | 1279 | | -21.467 | 47.142 | 1.00 19.97 | |
| MOTA | | | | | | | | | |
| ATOM | 8578 | С | CYS | 1279 | | -22.245 | 46.055 | 1.00 19.66 | |
| ATOM | 8579 | 0 | CYS | 1279 | | -22.019 | 44.881 | 1.00 18.47 | |
| MOTA | 8580 | N | LEU | 1280 | -11.294 | -21.530 | 46.738 | 1.00 18.36 | |
| ATOM | 8581 | CA | LEU | 1280 | -11.924 | -20.336 | 46.179 | 1.00 17.84 | |
| ATOM | 8582 | СВ | LEU | 1280 | | -20.059 | 46.814 | 1.00 19.49 | |
| | | | | | | -18.734 | 46.406 | 1.00 18.08 | |
| MOTA | 8583 | CG | LEU | 1280 | | | | | |
| MOTA | 8584 | | LEU | 1280 | | -18.712 | 44.897 | 1.00 19.62 | |
| ATOM | 8585 | CD2 | LEU | 1280 | -15.291 | -18.559 | 47.142 | 1.00 17.89 | |
| ATOM | 8586 | С | LEU | 1280 | -10.937 | -19.258 | 46.609 | 1.00 17.49 | |
| ATOM | 8587 | 0 | LEU | 1280 | -10.763 | -19.003 | 47.805 | 1.00 16.91 | |
| ATOM | 8588 | N | LEU | 1281 | | -18.634 | 45.636 | 1.00 17.29 | |
| | | | | | | -17.630 | | | |
| MOTA | 8589 | CA | LEU | 1281 | | | 45.930 | 1.00 16.61 | |
| MOTA | 8590 | CB | LEU | 1281 | | -17.969 | 45.147 | 1.00 16.66 | |
| ATOM | 8591 | CG | LEU | 1281 | -6.651 | -17.406 | 45.628 | 1.00 17.44 | |
| ATOM | 8592 | CD1 | LEU | 1281 | -5.524 | -18.159 | 44.929 | 1.00 15.28 | |
| MOTA | 8593 | | LEU | 1281 | -6.566 | -15.925 | 45.366 | 1.00 21.45 | |
| ATOM | 8594 | C | LEU | 1281 | | -16.195 | 45.633 | 1.00 17.29 | |
| | | | | | | | | 1.00 17.23 | |
| MOTA | 8595 | 0 | LEU | 1281 | | -15.825 | 44.475 | | |
| MOTA | 8596 | N | LEU | 1282 | | -15.398 | 46.689 | 1.00 16.41 | |
| ATOM | 8597 | CA | LEU | 1282 | -10.168 | -13.983 | 46.561 | 1.00 17.05 | |
| MOTA | 8598 | CB | LEU | 1282 | -11.093 | -13.534 | 47.699 | 1.00 16.06 | |
| MOTA | 8599 | CG | LEU | 1282 | -12,601 | -13.795 | 47.550 | 1.00 17.50 | |
| ATOM | 8600 | | LEU | 1282 | | -15.285 | 47.468 | 1.00 17.75 | |
| | | | | | | | | | |
| MOTA | 8601 | | LEU | 1282 | | -13.176 | 48.732 | 1.00 18.80 | |
| MOTA | 8602 | С | LEU | 1282 | | -13.169` | 46.635 | 1.00 17.94 | |
| ATOM | 8603 | 0 | LEU | 1282 | -8.030 | -13.425 | 47.487 | 1.00 22.05 | |
| MOTA | 8604 | N | ALA | 1283 | -8.712 | -12.199 | 45.744 | 1.00 14.13 | |
| ATOM | 8605 | CA | ALA | 1283 | | -11.363 | 45.771 | 1.00 14.02 | |
| | 8606 | | | 1283 | | -11.594 | 44.532 | 1.00 11.25 | |
| MOTA | | CB | ALA | | | | | | |
| MOTA | 8607 | C . | ALA | 1283 | -7.940 | -9.903 | 45.855 | 1.00 12.74 | |
| MOTA | 8608 | 0 | ALA | 1283 | -8.862 | -9.479 | 45.157 | 1.00 12.53 | |
| ATOM | 8609 | N | ASP | 1284 | -7.287 | -9.131 | 46.719 | 1.00 13.81 | |
| ATOM | 8610 | CA | ASP | 1284 | -7.623 | -7.718 | 46.827 | 1.00 14.31 | |
| MOTA | 8611 | CB | ASP | 1284 | -7.075 | -7.095 | 48.113 | 1.00 17.63 | |
| | 8612 | CG | ASP | 1284 | -7.972 | -7.298 | 49.310 | 1.00 19.26 | |
| MOTA | | | | | | | | | |
| ATOM | 8613 | | ASP | 1284 | -9.202 | -7.418 | 49.152 | 1.00 17.82 | |
| MOTA | 8614 | OD2 | ASP | 1284 | -7.428 | -7.301 | 50,430 | 1.00 23.10 | |
| MOTA | 8615 | C | ASP | 1284 | -7.003 | -6.912 | 45.702 | 1.00 15.99 | |
| MOTA | 8616 | 0 | ASP | 1284 | -5.930 | -7.256 | 45.202 | 1.00 14.33 | |
| ATOM | 8617 | N | LEU | 1285 | -7.688 | -5.849 | 45.290 | 1.00 13.28 | |
| ATOM | 8618 | CA | LEU | 1285 | -7.104 | -4.917 | 44.335 | 1.00 12.51 | |
| | | | | | | | | | |
| MOTA | 8619 | CB | LEU | 1285 | | | 43.418 | 1.00 14.13 | |
| ATOM | 8620 | CG | LEU | 1285 | -8.543 | -5.157 | 42.218 | | |
| MOTA | 8621 | CD1 | LEU | 1285 | -9.420 | -4.365 | 41.262 | 1.00 15.19 | |
| MOTA | 8622 | CD2 | LEU | 1285 | -7.273 | -5.633 | 41.508 | 1.00 15.66 | |
| ATOM | 8623 | С | LEU | 1285 | -6.616 | -3.907 | 45.373 | 1.00 13.60 | |
| ATOM | 8624 | Ŏ. | | 1285 | -7.386 | -3.463 | 46.225 | 1.00 13.40 | |
| | | | | | | | | | |
| ATOM | 8625 | N | PRO | 1286 | -5.319 | -3.569 | 45.349 | 1.00 13.01 | |
| MOTA | 8626 | CD | PRO | 1286 | -4.276 | -4.134 | 44.477 | 1.00 12.67 | |
| ATOM | 8627 | CA | PRO | 1286 | -4.751 | -2.621 | 46.312 | 1.00 13.67 | |
| MOTA | 8628 | CB | PRO | 1286 | -3.250 | -2.909 | 46.223 | 1.00 14.83 | |
| MOTA | 8629 | CG | PRO | 1286 | -3.075 | -3.237 | 44.758 | 1.00 13.00 | |
| ATOM | 8630 | C | PRO | 1286 | -5.079 | -1.147 | 46.079 | 1.00 13.64 | |
| | 8631 | o | PRO | 1286 | -5.772 | -0.781 | 45.128 | 1.00 14.01 | |
| ATOM | | | | | | | | 1.00 14.01 | |
| ATOM | 8632 | N | PHE | 1287 | -4.583 | -0.311 | 46.983 | | |
| MOTA | 8633 | CA | PHE | 1287 | -4.779 | 1.130 | 46.929 | 1.00 13.53 | |
| MOTA | 8634 | CB | PHE | 1287 | -3.805 | 1.782 | 47.915 | 1.00 15.05 | |
| MOTA | 8635 | CG | PHE | 1287 | -3.661 | 3.265 | 47.750 | 1.00 15.65 | - |
| ATOM | 8636 | | PHE | 1287 | -4.740 | 4.120 | 47.989 | 1.00 16.81 | |
| ATOM | 8637 | | PHE | 1287 | -2.435 | 3.814 | 47.372 | 1.00 13.49 | |
| | | | | | -4.593 | 5.490 | 47.865 | 1.00 16.89 | |
| ATOM | 8638 | | PHE | 1287 | | | | | |
| ATOM | 8639 | | PHE | 1287 | -2.281 | 5.184 | 47.247 | 1.00 14.29 | |
| ATOM | 8640 | CZ | PHE | 1287 | -3.367 | 6.032 | 47.492 | 1.00 17.50 | |
| MOTA | 8641 | С | PHE | 1287 | -4.587 | 1.692 | 45.515 | 1.00 14.14 | |
| ATOM | 8642 | 0 | PHE | 1287 | -3.581 | 1.418 | 44.851 | 1.00 11.80 | |
| ATOM | 8643 | N | MET | 1288 | -5.562 | 2.484 | 45.071 | 1.00 13.14 | |
| ATOM | 8644 | CA | MET | 1288 | -5.555 | 3.110 | 43.751 | 1.00 13.99 | |
| | | | | | | | | 1.00 15.56 | |
| MOTA | 8645 | CB | MET | 1288 | -4.470 | 4.198 | 43.687 | | |
| MOTA | 8646 | CG | MET | 1288 | -4.792 | 5.333 | 42.709 | 1.00 17.83 | |
| MOTA | 8647 | SD | MET | 1288 | -6.295 | | 43.134 | 1.00 16.61 | |
| ATOM | 8648 | CE | MET | 1288 | -5.573 | 7.644 | 44.077 | 1.00 17.67 | |
| MOTA | 8649 | С | MET | 1288 | -5.377 | 2.140 | 42.569 | 1.00 14.20 | |
| ATOM | 8650 | ō | MET | 1288 | -4.814 | 2.515 | 41.538 | 1.00 14.63 | |
| | | | | | -5.840 | 0.901 | 42.704 | 1.00 12.49 | |
| ATOM | 8651 | N | ALA | 1289 | | | | | |
| ATOM | 8652 | CA | ALA | 1289 | -5.723 | -0.046 | 41.596 | 1.00 13.64 | |
| | | | | | | | | | |

| ATOM | 8653 | CB | ALA | 1289 | -5.342 | -1.438 | 42.112 | 1.00 12.98 |
|--------|------|-----|-------|------|------------------|--------|--------|------------|
| ATOM | 8654 | С | ALA | 1289 | -7.039 | -0.117 | 40.821 | 1.00 12.89 |
| ATOM | 8655 | 0 | ALA | 1289 | -7.142 | -0.819 | 39.816 | 1.00 13.36 |
| ATOM | 8656 | N | TYR | 1290 | -8.045 | 0.623 | 41.276 | 1.00 11.64 |
| ATOM | 8657 | CA | TYR | 1290 | -9.347 | 0.624 | 40.605 | 1.00 12.12 |
| ATOM | 8658 | СВ | TYR | 1290 | -10.284 | -0.363 | 41.302 | 1.00 10.86 |
| | | CG | TYR | 1290 | -10.276 | -0.270 | 42.816 | 1.00 10.00 |
| ATOM | 8659 | | | | | | | |
| ATOM | 8660 | CD1 | | 1290 | -11.308 | 0.371 | 43.500 | 1.00 10.35 |
| ATOM | 8661 | CE1 | TYR | 1290 | -11.321 | 0.436 | 44.892 | 1.00 13.90 |
| ATOM | 8662 | CD2 | TYR | 1290 | -9.245 | -0.844 | 43.563 | 1.00 12.59 |
| MOTA | 8663 | CE2 | TYR | 1290 | -9.242 | -0.786 | 44.959 | 1.00 15.77 |
| MOTA | 8664 | CZ | TYR | 1290 | -10.290 | -0.144 | 45.616 | 1.00 16.49 |
| ATOM | 8665 | OH | TYR | 1290 | -10.313 | -0.095 | 46.992 | 1.00 16.97 |
| MOTA | 8666 | С | TYR | 1290 | -9.946 | 2.029 | 40:593 | 1.00 11.80 |
| MOTA | 8667 | 0 | TYR | 1290 | -11.142 | 2.212 | 40.811 | 1.00 12.18 |
| ATOM | 8668 | N | ALA | 1291 | -9.095 | 3.009 | 40.310 | 1.00 11.23 |
| ATOM | 8669 | CA | ALA | 1291 | -9.484 | 4.414 | 40.291 | 1.00 12.52 |
| ATOM | 8670 | CB | ALA | 1291 | -8.233 | 5.291 | 40.232 | 1.00 13.30 |
| MOTA | 8671 | C | ALA | 1291 | -10.425 | 4.748 | 39.141 | 1.00 13.87 |
| АТОМ . | 8672 | 0 | ALA | 1291 | -11.127 | 5.755 | 39.183 | 1.00 15.07 |
| ATOM | 8673 | N | THR | 1292 | -10.402 | 3.929 | 38.093 | 1.00 13.11 |
| ATOM | 8674 | CA | THR | 1292 | -11.295 | 4.111 | 36.953 | 1.00 13.77 |
| ATOM | 8675 | CB | THR | 1292 | -10.620 | 4.827 | 35.753 | 1.00 14.58 |
| | 8676 | | | 1292 | -9.685 | 3.944 | 35.733 | 1.00 13.37 |
| MOTA | | | THR | | -9.880 -9.880 | | | |
| MOTA | 8677 | CG2 | | 1292 | | 6.085 | 36.210 | 1.00 15.36 |
| ATOM | 8678 | С | THR | 1292 | -11.676 | 2.699 | 36.526 | 1.00 13.97 |
| ATOM | 8679 | 0 | THR | 1292 | -10.972 | 1.728 | 36.849 | 1.00 12.52 |
| MOTA | 8680 | N | PRO | 1293 | -12.805 | - 1 1 | 35.821 | 1.00 12.10 |
| ATOM | 8681 | CD | PRO | 1293 | -13.854 | 3.557 | 35.555 | 1.00 11.83 |
| MOTA | 8682 | CA | PRO | 1293 | -13.228 | 1.222 | 35.376 | 1.00 12.00 |
| MOTA | 8683 | CB | PRO | 1293 | -14.503 | 1.517 | 34.593 | 1.00 11.85 |
| ATOM | 8684 | CG | PRO - | 1293 | -15.078 | 2.695 | 35.378 | 1.00 11.15 |
| ATOM | 8685 | C · | PRO | 1293 | -12.138 | 0.577 | 34.518 | 1.00 14.03 |
| MOTA | 8686 | 0 | PRO | 1293 | -11.789 | -0.588 | 34.712 | 1.00 15.96 |
| ATOM | 8687 | N | GLU | 1294 | -11.592 | 1.351 | 33.585 | 1.00 14.44 |
| ATOM | 8688 | CA | GLU | 1294 | -10.533 | | 32.689 | 1.00 17.39 |
| ATOM | 8689 | СВ | GLU | 1294 | -10.024 | 2.047 | 31.836 | 1.00 20.55 |
| ATOM | 8690 | CG | GLU | 1294 | -8.898 | 1.708 | 30.876 | 1.00 28.83 |
| ATOM | 8691 | CD | GLU | 1294 | -8.043 | 2.922 | 30.527 | 1.00 32.90 |
| ATOM | 8692 | | GLU | 1294 | -7.124 | 3.253 | 31.311 | 1.00 36.01 |
| ATOM | 8693 | OE2 | | 1294 | -8.301 | 3.553 | 29.479 | 1.00 37.17 |
| | | | | | | | 33.471 | |
| ATOM | 8694 | C . | GLU | 1294 | -9.366 | 0.279 | | |
| ATOM | 8695 | 0 | GLU | 1294 | -8.904 | -0.828 | 33.179 | 1.00 15.04 |
| MOTA | 8696 | N · | GLN | 1295 | -8.873 | 1.011 | 34.462 | 1.00 15.47 |
| MOTA | 8697 | CA | GLN | 1295 | -7.760 | 0.500 | 35.257 | 1.00 15.54 |
| MOTA | 8698 | CB | GLN | 1295 | -7.184 | 1.609 | 36.133 | 1.00 16.24 |
| ATOM | 8699 | CG | GLN | 1295 | -6.427 | 2.633 | 35.322 | 1.00 23.28 |
| ATOM | 8700 | CD | GLN | 1295 | -6.020 | 3.825 | 36.139 | 1.00 24.86 |
| ATOM | 8701 | OE1 | GLN | 1295 | -5.407 | 3.679 | 37.192 | 1.00 24.58 |
| MOTA | 8702 | NE2 | GLN | 1295 | -6.356 | 5.021 | 35.656 | 1.00 26.69 |
| MOTA | 8703 | C · | GLN | 1295 | -8.182 | -0.682 | 36.106 | 1.00 13.96 |
| ATOM | 8704 | 0 | GLN | 1295 | -7.394 | -1.606 | 36.338 | 1.00 13.72 |
| ATOM | 8705 | N | ALA | 1296 | -9.424 | -0.654 | 36.576 | 1.00 13.84 |
| ATOM | 8706 | CA | ALA | 1296 | -9.936 | -1.755 | 37.377 | 1.00 13.08 |
| MOTA | 8707 | CB | ALA | 1296 | -11.364 | -1.452 | 37.848 | 1.00 14.56 |
| ATOM | 8708 | С | ALA | 1296 | -9.925 | -3.030 | 36.528 | 1.00 12.59 |
| ATOM | 8709 | 0 | ALA | 1296 | -9.525 | -4.083 | 37.010 | 1.00 13.75 |
| ATOM | 8710 | N | | 1297 | -10.345 | -2.934 | 35.265 | 1.00 10.91 |
| ATOM | 8711 | CA | PHE | 1297 | -10.363 | -4.121 | 34.399 | 1.00 11:05 |
| | | CB | PHE | 1297 | -10.886 | -3.819 | 32.985 | 1.00 9.65 |
| ATOM | 8712 | | | | | | | |
| ATOM | 8713 | CG | PHE | 1297 | -12.206 | -3.090 | 32.942 | 1.00 10.56 |
| ATOM | 8714 | | PHE | 1297 | -13.170 | -3.279 | 33.929 | 1.00 10.04 |
| ATOM | 8715 | CD2 | | 1297 | -12.475 | -2.205 | 31.898 | 1.00 11.57 |
| MOTA | 8716 | | PHE | 1297 | -14.387 | -2.593 | 33.891 | 1.00 10.32 |
| ATOM | 8717 | | PHE | 1297 | -13.684 | -1.513 | 31.840 | 1.00 13.36 |
| ATOM | 8718 | CZ | PHE | 1297 | -14.643 | -1.706 | 32.841 | 1.00 12.32 |
| ATOM | 8719 | С | PHE | 1297 | -8.956 | -4.698 | 34.240 | 1.00 10.73 |
| MOTA | 8720 | 0 | PHE | 1297 | -8.767 | -5.908 | 34.318 | 1.00 10.33 |
| MOTA | 8721 | N | GLU | 1298 | -7.981 | -3.827 | 33.998 | 1.00 10.95 |
| MOTA | 8722 | CA | GLU | 1298 | -6.607 | -4.265 | 33.799 | 1.00 12.53 |
| ATOM | 8723 | CB | GLU | 1298 | -5.736 | -3.091 | 33.353 | 1.00 16.83 |
| ATOM | 8724 | CG | GLU | 1298 | -4.361 | -3.499 | 32.848 | 1.00 24.35 |
| ATOM | 8725 | CD | GLU | 1298 | -4.377 | -3.908 | 31.382 | 1.00 28.25 |
| ATOM | 8726 | | GLU | 1298 | -5.089 | -4.875 | 31.025 | 1.00 30.56 |
| ATOM | 8727 | OE2 | | 1298 | -3.681 | -3.248 | 30.576 | 1.00 33.57 |
| MOTA | 8728 | C | GLU | 1298 | -5.990 | -4.913 | 35.036 | 1.00 11.29 |
| ATOM | 8729 | 0 | GLU | 1298 | -5.396 | -5.989 | 34.951 | 1.00 10.65 |
| | | - | | | 2.330 | 2.505 | | |

| ATOM | 8730 | N | ASN | 1299 | -6.130 | -4.274 | 36.190 | 1.00 10.85 |
|------|--------|-----|-----|------|---------|---------|--------|------------|
| ATOM | 8731 | CA | ASN | 1299 | -5.552 | -4.838 | 37.414 | 1.00 11.72 |
| ATOM | 8732 | CB | ASN | 1299 | -5.470 | -3.769 | 38.511 | 1.00 11.28 |
| ATOM | 8733 | CG | ASN | 1299 | -4.544 | -2.621 | 38.121 | 1.00 14.85 |
| ATOM | 8734 | OD1 | ASN | 1299 | -3.460 | -2.857 | 37.566 | 1.00 13.95 |
| ATOM | 8735 | ND2 | | 1299 | -4.944 | -1.389 | 38.413 | 1.00 13.47 |
| ATOM | 8736 | С | ASN | 1299 | -6.301 | -6.070 | 37.905 | 1.00 11.79 |
| ATOM | 8737 | ō | ASN | 1299 | -5.692 | -6.983 | 38,473 | 1.00 11.65 |
| MOTA | 8738 | N | ALA | 1300 | -7.619 | -6.104 | 37.701 | 1.00 11.62 |
| ATOM | 8739 | CA | ALA | 1300 | -8.384 | -7.281 | 38.095 | 1.00 9.62 |
| ATOM | 8740 | CB | ALA | 1300 | -9.864 | -7.042 | 37.911 | 1.00 11.93 |
| ATOM | 8741 | C | ALA | 1300 | -7.927 | -8.436 | 37.209 | 1.00 9.30 |
| ATOM | 8742 | 0 | ALA | 1300 | -7.725 | -9.552 | 37.688 | 1.00 11.63 |
| ATOM | 8743 | N | ALA | 1301 | -7.745 | -8.176 | 35.918 | 1.00 9.27 |
| ATOM | 8744 | CA | ALA | 1301 | -7.318 | -9.247 | 35.033 | 1.00 10.11 |
| ATOM | 8745 | CB | ALA | 1301 | -7.226 | -8.749 | 33.591 | 1.00 8.32 |
| ATOM | 8746 | С | ALA | 1301 | -5.981 | -9.807 | 35.492 | 1.00 10.42 |
| ATOM | 8747 | 0 | ALA | 1301 | -5.794 | -11.029 | 35.523 | 1.00 10.44 |
| ATOM | 8748 | N | THR | 1302 | -5.055 | -8.926 | 35.873 | 1.00 10.18 |
| ATOM | 8749 | CA | THR | 1302 | -3.729 | -9.378 | 36.312 | 1.00 10.80 |
| ATOM | 8750 | CB | THR | 1302 | -2.821 | -8.189 | 36.740 | 1.00 11.76 |
| ATOM | 8751 | OG1 | | 1302 | -2.586 | -7.327 | 35.612 | 1.00 12.59 |
| ATOM | 8752 | CG2 | | 1302 | -1.479 | -8.702 | 37.260 | 1.00 11.04 |
| ATOM | 8753 | С | THR | 1302 | -3.801 | -10.378 | 37.457 | 1.00 10.37 |
| ATOM | 8754 | 0 | THR | 1302 | -3.177 | -11.439 | 37.391 | 1.00 10.85 |
| ATOM | 8755 | N | VAL | 1303 | -4.563 | -10.070 | 38.502 | 1.00 9.66 |
| ATOM | 8756 | CA | VAL | 1303 | -4.622 | -10.991 | 39.630 | 1.00 9.50 |
| ATOM | 8757 | СВ | VAL | 1303 | -5.112 | -10.277 | 40.894 | 1.00 13.99 |
| ATOM | 8758 | | VAL | 1303 | -4.904 | -11.178 | 42.085 | 1.00 18.44 |
| ATOM | 8759 | | VAL | 1303 | -4.326 | -8.981 | 41.091 | 1.00 11.75 |
| ATOM | 8760 | С | VAL | 1303 | -5.440 | -12.253 | 39.358 | 1.00 10.29 |
| ATOM | 8761 | Ο. | VAL | 1303 | -5.187 | | 39.955 | 1.00 8.82 |
| ATOM | 8762 | N | MET | 1304 | -6.412 | -12.148 | 38.453 | 1.00 10.19 |
| MOTA | 8763 | CA | MET | 1304 | -7.219 | -13.307 | 38.069 | 1.00 12.39 |
| ATOM | 8764 | CB | MET | 1304 | -8.431 | -12.884 | 37.221 | 1.00 13.83 |
| MOTA | 8765 | CG | MET | 1304 | -9.485 | -12.065 | 37.951 | 1.00 18.90 |
| MOTA | 8766 | SD | MET | 1304 | -10.483 | -13.022 | 39.099 | 1.00 21.49 |
| MOTA | 8767 | CE | MET | 1304 | -11.599 | -13.972 | 37.916 | 1.00 17.14 |
| MOTA | 8768 | C | MET | 1304 | -6.345 | -14.277 | 37.254 | 1.00 11.47 |
| MOTA | 8769 | 0 | MET | 1304 | -6.400 | -15.495 | 37.462 | 1.00 11.55 |
| ATOM | 8770 | N | ARG | 1305 | -5.549 | -13.746 | 36.323 | 1.00 11.47 |
| MOTA | 8771 | CA | ARG | 1305 | -4.674 | -14.603 | 35.514 | 1.00 9.90 |
| ATOM | 8772 | CB | ARG | 1305 | -3.925 | -13.805 | 34.441 | 1.00 9.95 |
| MOTA | 8773 - | CG | ARG | 1305 | -4.805 | -13.184 | 33.373 | 1.00 13.47 |
| MOTA | 8774 | CD | ARG | 1305 | -4.001 | -12.850 | 32.131 | 1.00 13.07 |
| MOTA | 8775 | NE | ARG | 1305 | -4.782 | -12.012 | 31.231 | 1.00 18.31 |
| MOTA | 8776 | cz | ARG | 1305 | -4.895 | -10.694 | 31.343 | 1.00 17.19 |
| MOTA | 8777 | NH1 | ARG | 1305 | -4.261 | -10.044 | 32.317 | 1.00 17.95 |
| MOTA | 8778 | NH2 | ARG | 1305 | -5.680 | -10.033 | 30.500 | 1.00 16.90 |
| ATOM | 8779 | С | ARG | 1305 | -3.643 | -15.280 | 36.411 | 1.00 11.06 |
| MOTA | 8780 | 0 | ARG | 1305 | -3.161 | -16.370 | 36.103 | 1.00 10.28 |
| ATOM | 8781 | N | ALA | 1306 | -3.314 | -14.624 | 37.519 | 1.00 9.99 |
| MOTA | 8782 | CA | ALA | 1306 | -2.342 | -15.166 | 38.449 | 1.00 11.44 |
| ATOM | 8783 | CB | ALA | 1306 | -1.767 | -14.061 | 39.321 | 1.00 10.39 |
| MOTA | 8784 | C | ALA | 1306 | -2.919 | -16.278 | 39.319 | 1.00 12.44 |
| MOTA | 8785 | 0 | ALA | 1306 | -2.172 | -16.960 | 40.013 | 1.00 12.32 |
| MOTA | 8786 | N | GLY | 1307 | -4.238 | -16.455 | 39.297 | 1.00 12.27 |
| MOTA | 8787 | CA | GLY | 1307 | -4.823 | -17.529 | 40.075 | 1.00 13.76 |
| MOTA | 8788 | C | GLY | 1307 | -6.098 | -17.245 | 40.850 | 1.00 13.42 |
| MOTA | 8789 | 0 | GLY | 1307 | -6.733 | -18.176 | 41.345 | 1.00 14.10 |
| MOTA | 8790 | N | ALA | 1308 | -6.481 | -15.979 | 40.964 | 1.00 11.75 |
| MOTA | 8791 | CA | ALA | 1308 | -7.690 | -15.619 | 41.706 | 1.00 12.70 |
| MOTA | 8792 | CB | ALA | 1308 | -7.653 | -14.144 | 42.065 | 1.00 12.41 |
| MOTA | 8793 | С | ALA | 1308 | -8.984 | -15.939 | 40.958 | 1.00 12.62 |
| MOTA | 8794 | 0 | ALA | 1308 | | -15.996 | 39.725 | 1.00 12.19 |
| MOTA | 8795 | N | ASN | 1309 | -10.058 | -16.165 | 41.715 | 1.00 12.53 |
| MOTA | 8796 | CA | ASN | 1309 | -11.368 | -16.466 | 41.138 | 1.00 13.45 |
| MOTA | 8797 | CB | ASN | 1309 | -12.040 | | 41.852 | 1.00 14.86 |
| MOTA | 8798 | CG | ASN | 1309 | -11.249 | -18.914 | 41.769 | 1.00 15.09 |
| MOTA | 8799 | | ASN | 1309 | -10.999 | | 40.682 | 1.00 16.19 |
| MOTA | 8800 | | ASN | 1309 | -10.852 | -19.426 | 42.926 | 1.00 12.00 |
| MOTA | 8801 | С | ASN | 1309 | -12.288 | -15.271 | 41.323 | 1.00 13.77 |
| ATOM | 8802 | 0 | ASN | 1309 | -13.353 | -15.207 | 40.719 | 1.00 14.80 |
| MOTA | 8803 | N | MET | 1310 | | -14.332 | 42.165 | 1.00 13.61 |
| MOTA | 8804 | CA | MET | 1310 | -12.687 | | 42.491 | 1.00 12.31 |
| MOTA | 8805 | CB | MET | 1310 | | -13.584 | 43.562 | 1.00 14.22 |
| MOTA | 8806 | CG | MET | 1310 | -14.634 | -12.499 | 44.092 | 1.00 17.85 |

| ATOM | 8807 | SD | MET | 1310 | -15.747 | -13.199 | 45.346 | 1.00 | 20.90 |
|------|------|-----|-------|------|---------|---------|--------|------|-------|
| ATOM | 8808 | CE | MET | 1310 | -17.324 | -13.078 | 44.544 | 1.00 | 22.97 |
| ATOM | 8809 | С | MET | 1310 | | -12.051 | 43.016 | | 12.24 |
| ATOM | 8810 | ō | MET | 1310 | -10.737 | -12.304 | 43.589 | | 11.09 |
| ATOM | 8811 | N | VAL | 1311 | -12.227 | -10.816 | 42.818 | | 12.28 |
| | | | | 1311 | | | | | 13.29 |
| ATOM | 8812 | CA | VAL | | -11.466 | -9.666 | 43.272 | | |
| ATOM | 8813 | CB | VAL | 1311 | -11.215 | -8.728 | 42.088 | 1.00 | 15.81 |
| ATOM | 8814 | | VAL | 1311 | -10.651 | -7.421 | 42.566 | | 19.74 |
| MOTA | 8815 | CG2 | VAL | 1311 | -10.253 | -9.399 | 41.106 | | 16.21 |
| MOTA | 8816 | C | VAL | 1311 | -12.234 | -8.923 | 44.360 | 1.00 | 13.00 |
| MOTA | 8817 | 0 | VAL | 1311 | -13.462 | -8.831 | 44.303 | | 13.49 |
| ATOM | 8818 | N | LYS | 1312 | -11.519 | -8.409 | 45.355 | 1.00 | 12.33 |
| ATOM | 8819 | CA | LYS | 1312 | -12.158 | -7.642 | 46.413 | 1.00 | 11.16 |
| ATOM | 8820 | CB | LYS | 1312 | -11.806 | -8.197 | 47.797 | 1.00 | 13.10 |
| ATOM | 8821 | CG | LYS | 1312 | -12.465 | -7.402 | 48.925 | 1.00 | 15.32 |
| ATOM | 8822 | CD | LYS | 1312 | -12.623 | -8.211 | 50.207 | 1.00 | 16.26 |
| ATOM | 8823 | CE | LYS | 1312 | -11.297 | -8.393 | 50.927 | | 18.97 |
| ATOM | 8824 | NZ | LYS | 1312 | -10.732 | -7.084 | 51.357 | | 15.88 |
| ATOM | 8825 | С | LYS | 1312 | -11.716 | -6.188 | 46.315 | | 13.64 |
| ATOM | 8826 | 0 | LYS | | -10.526 | -5.897 | 46.172 | | 13.12 |
| ATOM | 8827 | N | ILE | 1313 | -12.680 | -5.274 | 46.381 | | 12.62 |
| | | | | | | -3.842 | 46.308 | | 14.45 |
| ATOM | 8828 | CA | ILE | 1313 | -12.388 | | | | |
| ATOM | 8829 | CB | ILE | 1313 | -12.802 | -3.250 | 44.949 | | 16.94 |
| ATOM | 8830 | CG2 | ILE | 1313 | -11.890 | -3.779 | 43.839 | | 19.34 |
| MOTA | 8831 | CG1 | ILE | 1313 | -14.266 | -3.588 | 44.661 | | 18.39 |
| MOTA | 8832 | CD1 | ILE | 1313 | -14.764 | -3.036 | 43.343 | | 19.90 |
| MOTA | 8833 | C | ILE | 1313 | -13.127 | -3.086 | 47.413 | 1.00 | 14.85 |
| MOTA | 8834 | Ю. | ILE | 1313 | -14.264 | -3.423 | 47.748 | 1.00 | 13.87 |
| MOTA | 8835 | N | GLU | 1314 | -12.483 | -2.054 | 47.951 | 1.00 | 15.54 |
| MOTA | 8836 | CA | GLU | 1314 | -13.047 | -1.259 | 49.043 | 1.00 | 14.90 |
| MOTA | 8837 | CB | GLU | 1314 | -11.944 | -0.825 | 50.019 | 1.00 | 16.10 |
| ATOM | 8838 | CG | GLU | 1314 | -11.092 | -1.946 | 50.573 | 1.00 | 17.92 |
| ATOM | 8839 | CD | GLŰ | 1314 | -9.990 | -1.445 | 51.512 | | 18.81 |
| ATOM | 8840 | OE1 | | 1314 | -9.869 | -0.218 | 51.713 | | 18.97 |
| ATOM | 8841 | OE2 | GLU | 1314 | -9.250 | -2.287 | 52.056 | | 20.27 |
| ATOM | 8842 | C | GLU | 1314 | -13.783 | -0.009 | 48.587 | | 14.25 |
| ATOM | 8843 | 0. | GLU | 1314 | -13.290 | 0.737 | 47.746 | | 16.21 |
| | | | | | -14.963 | 0.737 | 49.151 | | 16.28 |
| ATOM | 8844 | N | GLY | 1315 | | | 48.781 | | |
| ATOM | 8845 | CA | GLY | 1315 | -15.705 | 1.416 | | | 16.32 |
| ATOM | 8846 | C | GLY | 1315 | -17.196 | 1.197 | 48.692 | | 16.99 |
| ATOM | 8847 | 0 | GLY | 1315 | -17.662 | 0.060 | 48.630 | | 16.14 |
| ATOM | 8848 | N | GLY | 1316 | -17.942 | 2.295 | 48.669 | | 16.84 |
| ATOM | 8849 | CA | GLY | 1316 | -19.390 | 2.207 | 48.600 | | 18.58 |
| ATOM | 8850 | С | GLY | 1316 | -19.974 | 2.452 | 47.224 | | 19.09 |
| MOTA | 8851 | Ο. | GLY | 1316 | -19.491 | 1.928 | 46.222 | | 18.98 |
| ATOM | 8852 | N | GLU | 1317 | -21.022 | 3.268 | 47.196 | 1.00 | 19.78 |
| MOTA | 8853 | CA | GLU | 1317 | -21.753 | 3.608 | 45.983 | 1.00 | 21.03 |
| MOTA | 8854 | CB | GLU | 1317 | -22.791 | 4.686 | 46.302 | 1.00 | 24.13 |
| ATOM | 8855 | CG | GLU | 1317 | -24.226 | 4.206 | 46.235 | 1.00 | 34.04 |
| MOTA | 8856 | CD | GLU | 1317 | -24.910 | 4.591 | 44.946 | 1.00 | 35.84 |
| ATOM | 8857 | OE1 | | 1317 | -24.373 | 4.264 | 43.863 | 1.00 | 40.02 |
| ATOM | 8858 | OE2 | | 1317 | -25.986 | 5.219 | 45.018 | | 38.96 |
| MOTA | 8859 | C | GLU | 1317 | -20.948 | 4.052 | 44.768 | | 19.20 |
| ATOM | 8860 | ō | GLU | 1317 | -21.318 | 3.733 | 43.640 | 1.00 | |
| ATOM | 8861 | N | TRP | 1318 | -19.857 | 4.783 | 44.981 | | 17.44 |
| MOTA | 8862 | CA | TRP | 1318 | -19.079 | 5.258 | 43.846 | | 17.52 |
| ATOM | 8863 | CB | TRP | 1318 | -17.909 | 6.149 | 44.301 | | 18.44 |
| ATOM | 8864 | CG | TRP | 1318 | -16.754 | 5.430 | 44.951 | 1.00 | |
| | | | | | -15.534 | 5.018 | 44.316 | 1.00 | |
| ATOM | 8865 | CD2 | | 1318 | | 4.408 | 45.307 | 1.00 | |
| ATOM | 8866 | CE2 | | 1318 | -14.730 | | | | |
| ATOM | 8867 | | TRP | 1318 | -15.043 | 5.106 | 43.005 | 1.00 | |
| ATOM | 8868 | | TRP | 1318 | -16.645 | 5.060 | 46.262 | | 18.81 |
| MOTA | 8869 | | TRP | 1318 | -15.431 | 4.448 | 46.483 | | 17.06 |
| ATOM | 8870 | CZ2 | | 1318 | -13.458 | 3.888 | 45.030 | | 16.56 |
| ATOM | 8871 | CZ3 | | 1318 | -13.774 | 4.588 | 42.727 | 1.00 | |
| MOTA | 8872 | | TRP | 1318 | -13.000 | 3.987 | 43.736 | 1.00 | |
| MOTA | 8873 | С | TRP | 1318 | -18.557 | 4.121 | 42.972 | 1.00 | |
| ATOM | 8874 | 0 | TRP | 1318 | -18.168 | 4.346 | 41.830 | 1.00 | 17.22 |
| ATOM | 8875 | N | LEU | 1319 | -18.580 | 2.903 | 43.507 | 1.00 | 15.72 |
| MOTA | 8876 | CA | LEU | 1319 | -18.100 | 1.712 | 42.804 | 1.00 | 14.82 |
| MOTA | 8877 | СВ | LEU | 1319 | -17.556 | 0.698 | 43.813 | 1.00 | |
| ATOM | 8878 | CG | LEU | 1319 | -16.228 | 1.040 | 44.490 | 1.00 | |
| ATOM | 8879 | | LEU | 1319 | -15.872 | -0.036 | 45.504 | 1.00 | |
| ATOM | 8880 | | LEU | 1319 | -15.139 | 1.148 | 43.429 | | 14.65 |
| ATOM | 8881 | C | LEU | 1319 | -19.129 | 0.992 | 41.938 | 1.00 | |
| ATOM | 8882 | ō | LEU | 1319 | -18.779 | 0.080 | 41.192 | 1.00 | |
| ATOM | 8883 | N | VAL | 1320 | -20.393 | 1.385 | 42.028 | 1.00 | |
| 0.1 | 5505 | 7.4 | · 121 | 1020 | 20.22 | | | | |

| ATOM | 8884 | CA | VAL | 1320 | -2 | 1.446 | 0.700 | 41.274 | 1.00 15.61 |
|--------------|--------------|------------|------------|--------------|-----|----------------|------------------|------------------|--------------------------|
| ATOM | 8885 | СВ | VAL | 1320 | | 2.769 | 1.480 | 41.328 | 1.00 15.50 |
| ATOM | 8886 | CG1 | VAL | 1320 | -23 | 3.760 | 0.896 | 40.322 | 1.00 16.93 |
| ATOM | 8887 | CG2 | VAL | 1320 | -23 | 3.339 | 1.407 | 42.722 | 1.00 15.37 |
| MOTA | 8888 | C | VAL | 1320 | -2: | 1.114 | 0.401 | 39.819 | 1.00 15.88 |
| ATOM | 8889 | 0 | VAL | 1320 | -2: | 1.237 | -0.740 | 39.375 | 1.00 16.33 |
| MOTA | 8890 | N | GLU | 1321 | | 0.703 | 1.427 | 39.078 | 1.00 15.89 |
| ATOM | 8891 | CA | GLU | 1321 | | 0.367 | 1.256 | 37.667 | |
| MOTA | 8892 | CB | GLU | 1321 | | 9.982 | 2.601 | 37.038 | 1.00 18.42 |
| MOTA | 8893 | CG | GLU | 1321 | | 9.483 | 2.486 | 35.604 | 1.00 23.16 |
| MOTA | 8894 | CD | GLU | 1321 | | 9.156 | 3.836 | 34.967 | 1.00 27.92 |
| ATOM | 8895 | OE1 | | 1321 | | 3.295 | 4.576 | 35.495 | 1.00 28.97 |
| ATOM | 8896 | OE2 | | 1321 1321 | | 9.761 | 4.153 | 33.923 37.509 | 1.00 30.95 1.00 16.05 |
| ATOM | 8897 8898 | C O | GLU GLU | 1321 | | 9.212 | 0.265 -0.639 | 36.671 | 1.00 13.68 |
| ATOM ATOM | 8899 | N | THR | 1321 | | 3.180 | 0.441 | 38.325 | 1.00 13.47 |
| ATOM | 8900 | CA | THR | 1322 | | 7.013 | -0.432 | 38.271 | 1.00 14.01 |
| ATOM | 8901 | CB | THR | 1322 | | 5.983 | -0.025 | 39.352 | 1.00 14.03 |
| ATOM | 8902 | OG1 | THR | 1322 | | 5.481 | 1.280 | 39.046 | 1.00 16.65 |
| ATOM | 8903 | CG2 | THR | 1322 | | 4.807 | -1.001 | 39.395 | 1.00 13.60 |
| ATOM | 8904 | С | THR | 1322 | -17 | 7.432 | -1.887 | 38.462 | 1.00 11.93 |
| ATOM | 8905 | 0 | THR | 1322 | -1 | 7.064 | -2.768 | 37.675 | 1.00 13.98 |
| MOTA | 8906 | N | VAL | 1323 | | 3.221 | -2.133 | 39.501 | 1.00 12.13 |
| ATOM | 8907 | CA | VAL | 1323 | | 3.696 | -3.483 | 39.794 | 1.00 12.28 |
| MOTA | 8908 | CB | VAL | 1323 | | 9.511 | -3.508 | 41.107 | 1.00 14.17 |
| ATOM | 8909 | | VAL | 1323 | | 0.152 | -4.881 | 41.303 | 1.00 14.33 |
| ATOM | 8910 | CG2 | VAL | 1323 | | 3.597 | -3.177 | 42.275 | 1.00 12.26 |
| ATOM | 8911 | C | VAL | 1323 | | 9.537 | -4.061 | 38.647 | 1.00 13.33 1.00 13.70 |
| ATOM | 8912 | O N | VAL | 1323 1324 | | 9.326 0.480 | -5.203 -3.274 | 38.226 38.137 | 1.00 13.70 |
| ATOM ATOM | 8913 8914 | CA | GLN GLN | 1324 | | 1.322 | -3.274 | 37.039 | 1.00 15.37 |
| ATOM | 8915 | CB | GLN | 1324 | | 2.300 | -2.640 | 36.599 | 1.00 15.20 |
| ATOM | 8916 | CG | GLN | 1324 | | 3.292 | -2.224 | 37.682 | 1.00 22.21 |
| ATOM | 8917 | CD | GLN | 1324 | | 4.211 | -1.098 | 37.244 | 1.00 24.87 |
| ATOM | 8918 | OE1 | | 1324 | | 3.764 | -0.121 | 36.646 | 1.00 26.46 |
| ATOM | 8919 | NE2 | GLN | 1324 | -2 | 5.498 | -1.222 | 37.552 | 1.00 27.32 |
| ATOM | 8920 | C | GLN | 1324 | -20 | 0.460 | -4.149 | 35.850 | 1.00 15.72 |
| MOTA | 8921 | 0 | GLN | 1324 | | 0.617 | -5.237 | 35.304 | 1.00 14.44 |
| ATOM | 8922 | N | MET | 1325 | | 9.536 | -3.273 | 35.469 | 1.00 14.94 |
| ATOM | 8923 | CA | MET | 1325 | | 3.670 | -3.533 | 34.334 | 1.00 14.16 |
| ATOM | 8924 8925 | CB . CG | MET MET | 1325 1325 | | 7.942 3.877 | -2.251 -1.166 | 33.932 33.384 | 1.00 13.53 1.00 18.17 |
| ATOM ATOM | 8926 | SD | MET | 1325 | | 7.961 | 0.297 | 32.829 | 1.00 18.17 |
| ATOM | 8927 | CE | MET | 1325 | | 7.729 | -0.079 | 31.088 | 1.00 21.14 |
| ATOM | 8928 | c . | MET | 1325 | | 7.688 | -4.684 | 34.558 | 1.00 13.07 |
| ATOM | 8929 | 0 | MET | 1325 | | 7.438 | -5.465 | 33.639 | 1.00 12.98 |
| ATOM | 8930 | N | LEU | 1326 | -1 | 7.127 | -4.809 | 35.757 | 1.00 12.81 |
| ATOM | 8931 | CA | LEU | 1326 | -16 | 5.213 | -5.919 | 36.009 | 1.00 13.89 |
| MOTA | 8932 | CB | LEU | 1326 | -19 | 5.616 | -5.835 | 37.417 | 1.00 13.67 |
| MOTA | 8933 | CG | LEU | 1326 | | 4.431 | -4.878 | 37.574 | 1.00 14.23 |
| MOTA | 8934 | | LEU | 1326 | | 1.102 | -4.695 | 39.044 | 1.00 13.52 |
| ATOM | 8935 | | LEU | 1326 | | 3.228 | -5.438 | 36.815 | 1.00 13.49 |
| MOTA | 8936 | С | LEU | 1326 | | 5.965 | -7.235 | 35.864 | 1.00 15.09 1.00 17.34 |
| ATOM ATOM | 8937 8938 | O N | LEU THR | 1326 1327 | | 5.477 3.159 | -8.177 -7.292 | 35.229 36.453 | 1.00 17.34 |
| ATOM | 8939 | CA | THR | 1327 | | 3.993 | -8.495 | 36.420 | 1.00 17.21 |
| ATOM | 8940 | CB | THR | 1327 | | 0.327 | -8.284 | 37.203 | 1.00 17.21 |
| ATOM | 8941 | OG1 | | 1327 | | 0.041 | -8.025 | 38.585 | 1.00 22.00 |
| ATOM | 8942 | CG2 | | 1327 | | 1.203 | -9.530 | 37.120 | 1.00 21.12 |
| MOTA | 8943 | С | THR | 1327 | -19 | 9.331 | -8.944 | 34.999 | 1.00 17.87 |
| MOTA | 8944 | 0 | THR | 1327 | -19 | 9.200 | -10.123 | 34.673 | 1.00 15.79 |
| MOTA | 8945 | N | GLU | 1328 | | 9.763 | -8.018 | 34.146 | 1.00 19.35 |
| MOTA | 8946 | CA | GLU | 1328 | | 0.110 | -8.417 | 32.787 | 1.00 19.92 |
| ATOM | 8947 | CB | GLU | 1328 | | 0.951 | -7.330 | 32.104 | 1.00 24.09 |
| ATOM | 8948 | CG | GLU | 1328 | | 0.189 | -6.213 | 31.461 | 1.00 25.04 |
| ATOM | 8949 | CD OF1 | GLU | 1328 | | 1.115 2.172 | -5.173 -5.550 | 30.854 30.306 | 1.00 23.39 1.00 27.43 |
| ATOM ATOM | 8950 8951 | | GLU GLU | 1328 1328 | | 0.782 | -3.977 | 30.306 | 1.00 27.43 |
| ATOM | 8952 | C | GLU | 1328 | | 3.861 | -8.769 | 31.971 | 1.00 21.37 |
| ATOM | 8953 | Ö | GLU | 1328 | | 3.953 | -9.345 | 30.882 | 1.00 22.88 |
| ATOM | 8954 | N | ARG | 1329 | | 7.692 | -8.443 | 32.516 | 1.00 18.60 |
| ATOM | 8955 | CA | ARG | 1329 | | 5.425 | -8.760 | 31.870 | 1.00 16.07 |
| ATOM | 8956 | CB | ARG | 1329 | | 5.499 | -7.539 | 31.903 | 1.00 15.66 |
| ATOM | 8957 | CG | ARG | 1329 | | 5.916 | -6.473 | 30.899 | 1.00 12.22 |
| ATOM | 8958 | CD | ARG | 1329 | | 5.278 | -5.098 | 31.121 | 1.00 15.51 |
| ATOM | 8959 | NE | ARG | 1329 | | 5.805 | -4.147 | 30.144 | 1.00 11.85 |
| ATOM | 8960 | CZ | ARG | 1329 | -T. | 7.075 | -3.748 | 30.096 | 1.00 13.40 |
| | | | | | | | | | |

| ATOM | 8961 | NH1 | ARG | 1329 | -17.947 | -4.206 | 30.980 | 1.00 13.96 |
|--------------|--------------|-----------|------------|--------------|--------------------|------------------|------------------|--------------------------|
| ATOM | 8962 | NH2 | ARG | 1329 | -17.486 | -2.922 | 29.142 | 1.00 11.23 |
| MOTA | 8963 | С | ARG | 1329 | -15.737 | -9.986 | 32.496 | 1.00 16.04 |
| ATOM | 8964 | 0 | ARG | 1329 | -14.508 | -10.111 | 32.466 | 1.00 15.96 |
| ATOM | 8965 | N | ALA | 1330 | -16.541 | -10.872 | 33.078 | 1.00 15.89 |
| MOTA | 8966 | CA | ALA | 1330 | -16.060 | -12.129 | 33.678 | 1.00 14.56 |
| MOTA | 8967 | CB | ALA | 1330 | -15.213 | -12.897 | 32.650 | 1.00 14.48 |
| MOTA | 8968 | С | ALA | 1330 | -15.306 | -12.070 | 35.004 | 1.00 14.53 |
| MOTA | 8969 | 0 | ALA | 1330 | -14.685 | -13.053 | 35.409 | 1.00 14.82 |
| MOTA | 8970 | N | VAL | 1331 | -15.359 | -10.929 | 35.679 | 1.00 13.56 |
| MOTA | 8971 | CA | VAL | 1331 | | -10.779 | 36.951 | 1.00 14.03 |
| MOTA | 8972 | CB | VAL | 1331 | -13.755 | -9.536 | 36.926 | 1.00 14.54 |
| MOTA | 8973 | | VAL | 1331 | -13.126 | -9.306 | 38.300 | 1.00 15.64 |
| ATOM | 8974 | CG2 | VAL | 1331 | -12.653 | -9.736 | 35.888 | 1.00 17.69 |
| MOTA | 8975 | С | VAL | 1331 | | -10.663 | 38.117 | 1.00 13.93 |
| MOTA | 8976 | 0 | VAL | 1331 | -16.349 | -9.660 | 38.260 | 1.00 15.56 |
| ATOM | 8977 | N | PRO | 1332 | -15.779 | | 38.946 | 1.00 14.57 |
| MOTA | 8978 | CD | PRO | 1332 | | -13.080 | 38.790 | 1.00 12.80 |
| ATOM | 8979 | CA | PRO | 1332 | | -11.638 | 40.079 | 1.00 14.22 |
| MOTA | 8980 | CB | PRO | 1332 | | -13.077 | 40.572 | 1.00 15.61 |
| ATOM | 8981 | CG | PRO | 1332 | -15.500 | | 40.155 | 1.00 20.45 |
| ATOM | 8982 | C | PRO | 1332 | -16.111 | | 41.100 | 1.00 13.84 |
| ATOM | 8983 | 0 | PRO | 1332 | | -10.616 | 41.268 | 1.00 11.75 |
| ATOM | 8984 8985 | N CA | VAL VAL | 1333 1333 | -16.976 -16.502 | -9.966 -8.991 | 41.784 42.752 | 1.00 12.32 1.00 11.45 |
| ATOM | 8986 | CA CB | VAL | 1333 | -16.886 | -7.561 | 42.732 | 1.00 11.45 |
| ATOM ATOM | 8987 | CG1 | | 1333 | -16.465 | -6.551 | 43.378 | 1.00 10.38 |
| ATOM | 8988 | CG2 | VAL | 1333 | -16.228 | -7.235 | 40.987 | 1.00 12.00 |
| ATOM | 8989 | C | VAL | 1333 | -17.022 | -9.206 | 44.150 | 1.00 13.49 |
| ATOM | 8990 | o · | VAL | 1333 | -18.176 | -9.581 | 44.346 | 1.00 13.43 |
| ATOM | 8991 | N | CYS | 1334 | -16.145 | -8.987 | 45.122 | 1.00 12.49 |
| ATOM | 8992 | CA | CYS | 1334 | -16.515 | -9.072 | 46.524 | 1.00 13.08 |
| ATOM | 8993 | CB | CYS | 1334 | -15.561 | -9.988 | 47.294 | 1.00 14.71 |
| ATOM | 8994 | SG | CYS | 1334 | -15.827 | -9.940 | 49.091 | 1.00 15.45 |
| ATOM | 8995 | С | CYS | 1334 | -16.359 | -7.637 | 47.015 | 1.00 13.95 |
| ATOM | 8996 | 0 | CYS | 1334 | -15.312 | -7.011 | 46.818 | 1.00 14.76 |
| ATOM | 8997 | N | GLY | 1335 | -17.413 | -7.114 | 47.627 | 1.00 14.01 |
| ATOM | 8998 | CA | GLY | 1335 | -17.373 | -5.764 | 48.141 | 1.00 13.56 |
| ATOM | 8999 | С | GLY | 1335 | -16.726 | -5.747 | 49.510 | 1.00 -13.93 |
| ATOM | 9000 | 0 | GLY | 1335 | -16.501 | -6.802 | 50.105 | 1.00 14.54 |
| ATOM | 9001 | N | HIS | 1336 | -16.445 | -4.551 | 50.017 | 1.00 14.71 |
| ATOM | 9002 | CA | HIS | 1336 | -15.801 | -4.397 | 51.320 | 1.00 14.53 |
| ATOM | 9003 | CB | HIS | 1336 | -14.277 | -4.469 | 51.143 | 1.00 13.80 |
| MOTA | 9004 | CG | HIS | 1336 | -13.511 | -4.501 | 52.431 | 1.00 16.43 |
| MOTA | 9005 | CD2 | | 1336 | -13.866 | -4.166 | 53.697 | 1.00 14.92 |
| ATOM | 9006 | ND1 | | 1336 | -12.199 | -4.917 | 52.502 | 1.00 16.33 |
| ATOM | 9007 | CE1 | | 1336 | -11.778 | -4.839 | 53.752 | 1.00 17.68 |
| MOTA | 9008 | | HIS | 1336 | -12.769 | -4.386 | 54.498 | 1.00 15.76 |
| ATOM | 9009 | C | HIS | 1336 | -16.206 | -3.043 | 51.905 | 1.00 14.17 |
| ATOM | 9010 | 0 | HIS | 1336 | -15.852 | -2.005 | 51.363 | 1.00 13.31 |
| ATOM | 9011 | N | LEU | 1337 | -16.947 | -3.069 -1.855 | 53.010 | 1.00 16.38 |
| ATOM | 9012 | CA | LEU | 1337 | -17.417 | | 53.662 | 1.00 14.42 |
| ATOM | 9013 | CB | LEU | 1337 | -18.937 | -1.727 | 53.509 | 1.00 14.97 |
| ATOM | 9014 | CG CD1 | LEU | 1337 | -19.500 -21.022 | -1.425 | 52.118 52.174 | 1.00 13.18 1.00 16.54 |
| ATOM | 9015 9016 | CD2 | LEU LEU | 1337 1337 | -19.039 | -1.498 -0.057 | 51.659 | 1.00 15.16 |
| ATOM ATOM | 9017 | CDZ | LEU | 1337 | -17.074 | -1.819 | 55.152 | 1.00 15.10 |
| ATOM | 9018 | 0 | LEU | 1337 | -16.704 | -2.835 | 55.735 | 1.00 15.49 |
| ATOM | 9019 | N | GLY | 1338 | -17.234 | -0.646 | 55.763 | 1.00 16.52 |
| ATOM | 9020 | ĊA | GLY | 1338 | -16.931 | -0.487 | 57.175 | 1.00 18.65 |
| ATOM | 9021 | C | GLY | 1338 | -15.546 | 0.103 | 57.329 | 1.00 20.37 |
| ATOM | 9022 | ō | GLY | 1338 | -15.244 | 1.169 | 56.779 | 1.00 20.72 |
| ATOM | 9023 | N | LEU | 1339 | -14.692 | -0.592 | 58.071 | 1.00 21.08 |
| ATOM | 9024 | CA | LEU | 1339 | -13.328 | -0.130 | 58.274 | 1.00 21.80 |
| ATOM | 9025 | СВ | LEU | 1339 | -12.760 | -0.690 | 59.586 | 1.00 22.96 |
| MOTA | 9026 | CG | LEU | 1339 | -11.636 | 0.099 | 60.273 | 1.00 26.11 |
| ATOM | 9027 | CD1 | LEU | 1339 | -11.099 | -0.714 | 61.435 | 1.00 25.23 |
| MOTA | 9028 | CD2 | | 1339 | -10.528 | 0.410 | 59.290 | 1.00 25.89 |
| MOTA | 9029 | С | LEU | 1339 | -12.500 | -0.633 | 57.096 | 1.00 21.63 |
| MOTA | 9030 | 0 | LEU | 1339 | -12.007 | -1.762 | 57.108 | 1.00 21.30 |
| ATOM | 9031 | N | THR | 1340 | -12.386 | 0.205 | 56.070 | 1.00 21.68 |
| MOTA | 9032 | CA | THR | 1340 | -11.618 | -0.104 | 54.864 | 1.00 22.62 |
| MOTA | 9033 | CB | THR | 1340 | -12.301 | 0.507 | 53.626 | 1.00 23.97 |
| MOTA | 9034 | OG1 | THR | 1340 | -12.526 | 1.906 | 53.842 | 1.00 23.53 |
| ATOM | 9035 | | THR | 1340 | -13.641 | -0.169 | 53.375 | 1.00 26.26 |
| ATOM | 9036 | С | THR | 1340 | -10.232 | 0.510 | 55.053 | 1.00 20.26 |
| ATOM | 9037 | 0 | THR | 1340 | -10.057 | 1.715 | 54.899 | 1.00 23.50 |
| | | | | | | | | |

| MOTA | 9038 | N | PRO | 1341 | -9.226 | -0.323 | 55.372 | 1.00 20.57 |
|--------|------|-----------|-----|------|---------|--------|--------|------------|
| MOTA | 9039 | CD | PRO | 1341 | -9.300 | -1.794 | 55.327 | 1.00 21.40 |
| MOTA | 9040 | CA | PRO | 1341 | -7.842 | 0.114 | 55.603 | 1.00 19.00 |
| ATOM | 9041 | CB | PRO | 1341 | -7.091 | -1.205 | 55.802 | 1.00 22.07 |
| ATOM | 9042 | CG | PRO | 1341 | -7.881 | -2.171 | 54.978 | 1.00 25.73 |
| ATOM | 9043 | C | PRO | 1341 | -7.180 | 1.019 | 54.570 | 1.00 18.31 |
| | 9044 | ō | PRO | 1341 | -6.332 | 1.832 | 54.928 | 1.00 16.70 |
| ATOM | | | | | | | | |
| ATOM | 9045 | N | GLN | 1342 | -7.551 | 0.895 | 53.299 | |
| ATOM | 9046 | CA | GLN | 1342 | -6.944 | 1.751 | 52.284 | 1.00 18.99 |
| ATOM | 9047 | CB | GLN | 1342 | -7.432 | 1.355 | 50.882 | 1.00 16.29 |
| ATOM | 9048 | CG | GLN | 1342 | -6.722 | 0.124 | 50.316 | 1.00 17.70 |
| ATOM | 9049 | CD | GLN | 1342 | -7.365 | -0.407 | 49.047 | 1.00 18.63 |
| ATOM | 9050 | OE1 | GLN | 1342 | -7.891 | 0.360 | 48.236 | 1.00 21.48 |
| ATOM | 9051 | NE2 | GLN | 1342 | -7.310 | -1.725 | 48.858 | 1.00 20.30 |
| ATOM | 9052 | С | GLN | 1342 | -7.225 | 3.235 | 52.559 | 1.00 18.46 |
| ATOM | 9053 | ō | GLN | 1342 | -6.435 | 4.104 | 52.189 | 1.00 20.27 |
| ATOM | 9054 | N | SER | 1343 | -8.347 | 3.528 | 53.207 | 1.00 20.86 |
| | 9055 | CA | SER | 1343 | -8.684 | 4.913 | 53.528 | 1.00 21.17 |
| ATOM | | | | | | | | |
| ATOM | 9056 | CB | SER | 1343 | -10.190 | 5.154 | 53.330 | 1.00 22.94 |
| MOTA | 9057 | OG | SER | 1343 | -10.574 | 4.937 | 51.979 | 1.00 24.54 |
| ATOM | 9058 | С | SER | 1343 | -8.288 | 5.261 | 54.972 | 1.00 21.41 |
| ATOM | 9059 | 0 | SER | 1343 | -8.924 | 6.099 | 55.620 | 1.00 20.45 |
| ATOM | 9060 | N | VAL | 1344 | -7.232 | 4.632 | 55.480 | 1.00 20.55 |
| ATOM | 9061 | CA | VAL | 1344 | -6.802 | 4.911 | 56.849 | 1.00 21.71 |
| ATOM | 9062 | СВ | VAL | 1344 | -5.552 | 4.060 | 57.252 | 1.00 23.85 |
| ATOM | 9063 | | VAL | 1344 | -4.370 | 4.379 | 56.351 | 1.00 21.50 |
| | 9064 | | VAL | 1344 | -5.201 | 4.321 | 58.712 | 1.00 22.91 |
| ATOM | | | | | | 6.398 | | |
| ATOM | 9065 | С | VAL | 1344 | -6.501 | | 57.057 | 1.00 22.37 |
| ATOM | 9066 | 0 | VAL | 1344 | -6.803 | 6.960 | 58.114 | 1.00 22.26 |
| MOTA | 9067 | N | ASN | 1345 | -5.929 | 7.038 | 56.041 | 1.00 22.04 |
| ATOM | 9068 | CA | ASN | 1345 | -5.596 | 8.458 | 56.123 | 1.00 22.35 |
| ATOM | 9069 | CB | ASN | 1345 | -4.665 | 8.845 | 54.974 | 1.00 22.83 |
| MOTA | 9070 | CG | ASN | 1345 | -3.349 | 8.103 | 55.030 | 1.00 22.33 |
| ATOM | 9071 | OD1 | | 1345 | -2.566 | 8.288 | 55.958 | 1.00 23.07 |
| ATOM | 9072 | ND2 | | 1345 | -3.103 | 7.248 | 54.045 | 1.00 22.68 |
| ATOM | 9073 | C | ASN | 1345 | -6.840 | 9.336 | 56.103 | 1.00 24.24 |
| | | | | | | 10.465 | 56.588 | 1.00 23.31 |
| ATOM | 9074 | 0 | ASN | 1345 | -6.816 | | - | |
| ATOM | 9075 | N | ILE | 1346 | -7.923 | 8.817 | 55.534 | 1.00 24.67 |
| MOTA | 9076 | CA | ILE | 1346 | -9.179 | 9.561 | 55.477 | 1.00 26.60 |
| MOTA | 9077 | CB | ILE | 1346 | -10.155 | 8.949 | 54.447 | 1.00 25.22 |
| ATOM | 9078 | CG2 | ILE | 1346 | -11.529 | 9.593 | 54.580 | 1.00 25.45 |
| ATOM | 9079 | CG1 | ILE | 1346 | -9.604 | 9.121 | 53.031 | 1.00 26.82 |
| ATOM | 9080 | CD1 | ILE | 1346 | -9.646 | 10.548 | 52.518 | 1.00 27.54 |
| ATOM | 9081 | С | ILE | 1346 | -9.847 | 9.534 | 56.850 | 1.00 25.86 |
| ATOM | 9082 | 0. | ILE | 1346 | -10.311 | 10.565 | 57.337 | 1.00 27.66 |
| ATOM | 9083 | N | PHE | 1347 | -9.896 | 8.352 | 57.463 | 1.00 26.34 |
| ATOM | 9084 | CA | PHE | 1347 | -10.513 | 8.180 | 58.780 | 1.00 27.79 |
| | | | | 1347 | -10.855 | 6.707 | 59.040 | 1.00 30.55 |
| ATOM | 9085 | CB | PHE | | | | | |
| ATOM | 9086 | CG | PHE | 1347 | -11.662 | 6.055 | 57.951 | 1.00 33.41 |
| MOTA | 9087 | | PHE | 1347 | -12.751 | 6.707 | 57.382 | 1.00 33.70 |
| ATOM | 9088 | CD2 | PHE | 1347 | -11.349 | 4.766 | 57.518 | 1.00 34.68 |
| ATOM | 9089 | CE1 | PHE | 1347 | -13.516 | 6.088 | 56.398 | 1.00 34.26 |
| MOTA | 9090 | CE2 | PHE | 1347 | -12.108 | 4.137 | 56.533 | 1.00 34.13 |
| MOTA | 9091 | CZ | PHE | 1347 | -13.193 | 4.799 | 55.973 | 1.00 35.64 |
| MOTA | 9092 | C | PHE | 1347 | -9.609 | 8.655 | 59.912 | 1.00 28.04 |
| ATOM | 9093 | 0 | PHE | 1347 | -10.062 | 8.822 | 61.044 | 1.00 25.56 |
| ATOM | 9094 | N | GLY | 1348 | -8.329 | 8.852 | 59.609 | 1.00 28.73 |
| ATOM | 9095 | CA | GLY | 1348 | -7.387 | 9.290 | 60.625 | 1.00 30.19 |
| | | | | | | | | |
| ATOM | 9096 | С | GLY | 1348 | -6.961 | 8.147 | 61.531 | |
| ATOM | 9097 | 0 | GLY | 1348 | -6.574 | 8.361 | 62.679 | 1.00 32.36 |
| MOTA | 9098 | N | GLY | 1349 | -7.039 | 6.923 | 61.019 | 1.00 32.22 |
| ATOM | 9099 | CA | GLY | 1349 | -6.651 | 5.770 | 61.812 | 1.00 33.19 |
| ATOM | 9100 | C | GLY | 1349 | -7.580 | 4.592 | 61.597 | 1.00 34.56 |
| ATOM | 9101 | 0 | GLY | 1349 | -8.482 | 4.649 | 60.762 | 1.00 32.55 |
| ATOM | 9102 | N | TYR | 1350 | -7.359 | 3.517 | 62.346 | 1.00 35.88 |
| ATOM . | 9103 | CA | TYR | 1350 | -8.195 | 2.333 | 62.226 | 1.00 36.67 |
| ATOM | 9104 | CB | TYR | 1350 | -7.336 | 1.069 | 62.293 | 1.00 36.59 |
| | | | | | -6.220 | 1.046 | 61.271 | 1.00 38.85 |
| ATOM | 9105 | CG CD1 | TYR | 1350 | | | | 1.00 38.83 |
| ATOM | 9106 | CD1 | TYR | 1350 | -4.989 | 1.643 | 61.542 | |
| ATOM | 9107 | CE1 | TYR | 1350 | -3.969 | 1.661 | 60.592 | 1.00 38.99 |
| ATOM | 9108 | CD2 | TYR | 1350 | -6.406, | 0.463 | 60.017 | 1.00 38.83 |
| ATOM | 9109 | CE2 | TYR | 1350 | -5.389 | 0.478 | 59.054 | 1.00 38.92 |
| MOTA | 9110 | CZ | TYR | 1350 | -4.177 | 1.079 | 59.350 | 1.00 38.88 |
| ATOM | 9111 | OH | TYR | 1350 | -3.174 | 1.117 | 58.407 | 1.00 38.09 |
| ATOM | 9112 | С | TYR | 1350 | -9.239 | 2.327 | 63.336 | 1.00 37.58 |
| ATOM | 9113 | ō | TYR | 1350 | -9.110 | 1.612 | 64.330 | 1.00 38.34 |
| ATOM | 9114 | N | LYS | 1351 | -10.278 | 3.132 | 63.150 | 1.00 37.80 |
| | | ** | | | • | | | |

| ATOM | 9115 | CA | LYS | 1351 | -11.349 | 3.254 | 64.128 | 1.00 37.85 |
|------|------|--------|-----|------|---------|--------|--------|------------|
| ATOM | 9116 | СВ | LYS | 1351 | -11.650 | 4.738 | 64.354 | 1.00 39.96 |
| MOTA | 9117 | CG | LYS | 1351 | -10.399 | 5.592 | 64.529 | 1.00 41.93 |
| | | | | | | | | |
| ATOM | 9118 | CD | LYS | 1351 | -10.671 | 7.063 | 64.253 | 1.00 43.31 |
| MOTA | 9119 | CE | LYS | 1351 | -9.373 | 7.860 | 64.209 | 1.00 44.78 |
| MOTA | 9120 | NZ | LYS | 1351 | -9.596 | 9.288 | 63.846 | 1.00 44.41 |
| ATOM | 9121 | С | LYS | 1351 | -12.612 | 2.531 | 63.648 | 1.00 37.02 |
| MOTA | 9122 | 0 | LYS | 1351 | -12.809 | 2.329 | 62.449 | 1.00 35.65 |
| ATOM | 9123 | N | VAL | 1352 | -13.461 | 2.145 | 64.595 | 1.00 36.10 |
| ATOM | 9124 | CA | VAL | 1352 | -14.705 | 1.456 | 64.280 | 1.00 35.05 |
| ATOM | 9125 | CB | VAL | 1352 | -15.483 | 1.100 | 65.569 | 1.00 35.70 |
| ATOM | 9126 | | VAL | 1352 | -16.731 | 0.303 | 65.232 | 1.00 34.09 |
| ATOM | 9127 | CG2 | VAL | 1352 | -14.586 | 0.314 | 66.512 | 1.00 35.71 |
| | 9128 | C | VAL | 1352 | -15.570 | 2.358 | 63.405 | 1.00 34.29 |
| ATOM | | | | | | | | |
| MOTA | 9129 | 0 | VAL | 1352 | -15.604 | 3.576 | 63.595 | 1.00 32.86 |
| MOTA | 9130 | N | GLN | 1353 | -16.259 | 1.755 | 62.441 | 1.00 33.15 |
| MOTA | 9131 | CA | GLN | 1353 | -17.121 | 2.493 | 61.523 | 1.00 33.61 |
| ATOM | 9132 | CB | GLN | 1353 | -16.664 | 2.248 | 60.082 | 1.00 35.20 |
| MOTA | 9133 | CG | GLN | 1353 | -16.394 | 3.503 | 59.269 | 1.00 37.01 |
| ATOM | 9134 | CD | GLN | 1353 | -15.374 | 4.407 | 59.920 | 1.00 37.73 |
| MOTA | 9135 | OE1 | GLN | 1353 | -14.339 | 3.948 | 60.405 | 1.00 39.42 |
| MOTA | 9136 | NE2 | | 1353 | -15.656 | 5.703 | 59.929 | 1.00 39.06 |
| ATOM | 9137 | C | GLN | 1353 | -18.568 | 2.038 | 61.678 | 1.00 32.00 |
| ATOM | | | | 1353 | -18.839 | 1.006 | 62.289 | 1.00 32.23 |
| | 9138 | 0 | GLN | | | | | |
| ATOM | 9139 | N | GLY | 1354 | -19.497 | 2.810 | 61.124 | 1.00 32.12 |
| MOTA | 9140 | CA | GLY | 1354 | -20.901 | 2.445 | 61.207 | 1.00 32.69 |
| MOTA | 9141 | С | GLY | 1354 | -21.624 | 2.931 | 62.453 | 1.00 33.83 |
| MOTA | 9142 | 0 | GLY | 1354 | -22.812 | 2.658 | 62.634 | 1.00 33.12 |
| MOTA | 9143 | N | ARG | 1355 | -20.912 | 3.646 | 63.317 | 1.00 33.73 |
| ATOM | 9144 | CA | ARG | 1355 | -21.509 | 4.168 | 64.538 | 1.00 35.35 |
| ATOM | 9145 | СВ | ARG | 1355 | -20.420 | 4.610 | 65.523 | 1.00 36.22 |
| ATOM | 9146 | CG | ARG | 1355 | -19.601 | 3.469 | 66.116 | 1.00 37.99 |
| ATOM | 9147 | CD | ARG | 1355 | -19.623 | 3.530 | 67.636 | 1.00 37.53 |
| ATOM | 9148 | NE | ARG | 1355 | -18.923 | 2.412 | 68.266 | 1.00 38.27 |
| | | | | | | 2.278 | 68.305 | 1.00 37.61 |
| ATOM | 9149 | CZ | ARG | 1355 | -17.601 | | | |
| ATOM | 9150 | NH1 | | 1355 | -16.819 | 3.195 | 67.752 | 1.00 38.90 |
| MOTA | 9151 | NH2 | | 1355 | -17.062 | 1.228 | 68.905 | 1.00 38.50 |
| ATOM | 9152 | C | ARG | 1355 | -22.417 | 5.353 | 64.221 | 1.00 34.99 |
| MOTA | 9153 | 0 | ARG | 1355 | -21.988 | 6.326 | 63.601 | 1.00 33.87 |
| MOTA | 9154 | N | GLY | 1356 | -23.673 | 5.268 | 64.645 | 1.00 35.30 |
| ATOM | 9155 | CA | GLY | 1356 | -24.603 | 6.353 | 64.388 | 1.00 36.39 |
| ATOM | 9156 | С | GLY | 1356 | -25.609 | 5.991 | 63.316 | 1.00 36.56 |
| ATOM | 9157 | 0 | GLY | 1356 | -25.403 | 5.044 | 62.556 | 1.00 37.08 |
| MOTA | 9158 | N | ASP | 1357 | -26.704 | 6.741 | 63.251 | 1.00 35.94 |
| ATOM | 9159 | CA | ASP | 1357 | -27.730 | 6.470 | 62.257 | 1.00 35.55 |
| ATOM | 9160 | CB | ASP | 1357 | -29.029 | 7.206 | 62.596 | 1.00 38.36 |
| | | | | | | | | |
| MOTA | 9161 | CG | ASP | 1357 | -29.677 | 6.687 | 63.863 | 1.00 39.91 |
| MOTA | 9162 | | ASP | 1357 | -29.647 | 5.458 | 64.092 | 1.00 41.41 |
| ATOM | 9163 | | ASP | 1357 | -30.229 | 7.504 | 64.624 | 1.00 42.41 |
| MOTA | 9164 | C | ASP | 1357 | -27.280 | 6.860 | 60.859 | 1.00 33.61 |
| MOTA | 9165 | 0 | ASP | 1357 | -27.444 | 6.092 | 59.915 | 1.00 34.09 |
| MOTA | 9166 | N | GLU | 1358 | -26.710 | 8.051 | 60.723 | 1.00 31.82 |
| ATOM | 9167 | CA | GLU | 1358 | -26.257 | 8.517 | 59.419 | 1.00 32.56 |
| MOTA | 9168 | СВ | GLU | 1358 | -25.702 | 9.938 | 59.531 | 1.00 35.82 |
| ATOM | 9169 | CG | GLU | 1358 | -25.286 | 10.550 | 58.206 | 1.00 41.80 |
| ATOM | 9170 | CD | GLU | 1358 | -24.844 | 11.992 | 58.347 | 1.00 44.28 |
| ATOM | 9171 | | GLU | 1358 | -25.675 | 12.835 | 58.748 | 1.00 47.82 |
| | | | | | | | 58.062 | 1.00 47.55 |
| ATOM | 9172 | | GLU | 1358 | -23.665 | 12.286 | | |
| ATOM | 9173 | С | GLU | 1358 | -25.203 | 7.584 | 58.819 | 1.00 31.25 |
| MOTA | 9174 | 0 | GLU | 1358 | -25.300 | 7.199 | 57.652 | 1.00 29.54 |
| MOTA | 9175 | N | ALA | 1359 | -24.205 | 7.218 | 59.619 | 1.00 28.61 |
| MOTA | 9176 | CA | ALA | 1359 | -23.141 | 6.327 | 59.162 | 1.00 26.73 |
| ATOM | 9177 | CB | ALA | 1359 | -22.033 | 6.251 | 60.213 | 1.00 27.02 |
| ATOM | 9178 | С. | ALA | 1359 | -23.694 | 4.931 | 58.887 | 1.00 25.02 |
| ATOM | 9179 | 0 | ALA | 1359 | -23.314 | 4.281 | 57.910 | 1.00 25.54 |
| ATOM | 9180 | N | GLY | 1360 | -24.591 | 4.483 | 59.759 | 1.00 22.90 |
| ATOM | 9181 | CA | GLY | 1360 | -25.191 | 3.171 | 59.606 | 1.00 22.42 |
| ATOM | 9182 | C | GLY | 1360 | -26.036 | 3.070 | 58.350 | 1.00 23.63 |
| ATOM | 9183 | | GLY | 1360 | -25.874 | 2.143 | 57.552 | 1.00 21.50 |
| | | O N | | | -26.940 | 4.029 | 58.175 | 1.00 21.30 |
| MOTA | 9184 | N | ASP | 1361 | | | | |
| ATOM | 9185 | CA | ASP | 1361 | -27.809 | 4.055 | 57.010 | 1.00 24.97 |
| MOTA | 9186 | CB | ASP | 1361 | -28.776 | 5.242 | 57.082 | 1.00 25.15 |
| ATOM | 9187 | CG | ASP | 1361 | -29.778 | 5.109 | 58.212 | 1.00 25.98 |
| ATOM | 9188 | | ASP | 1361 | -30.037 | 3.963 | 58.634 | 1.00 24.04 |
| ATOM | 9189 | OD2 | ASP | 1361 | -30.312 | 6.148 | 58.662 | 1.00 26.75 |
| ATOM | 9190 | С | ASP | 1361 | -27.001 | 4.128 | 55.715 | 1.00 24.67 |
| ATOM | 9191 | 0 | ASP | 1361 | -27.418 | 3.599 | 54.682 | 1.00 23.97 |
| | | | | | | | | |

| ATOM | 9192 | N | GLN | 1362 | -25.843 | 4.775 | 55.763 | 1.00 23.06 |
|--------------|--------------|----------|------------|--------------|--------------------|------------------|------------------|--------------------------|
| ATOM | 9193 | CA | GLN | 1362 | -25.021 | 4.882 | 54.563 | 1.00 23.44 |
| ATOM | 9194 | CB | GLN | 1362 | -23.890 | 5.896 | 54.766 | 1.00 23.04 |
| ATOM | 9195 | CG | GLN | 1362 | -23.177 | 6.276 | 53.474 | 1.00 25.55 |
| ATOM | 9196 | CD | GLN | 1362 | -24.113 | 6.925 | 52.464 | 1.00 29.06 |
| ATOM | 9197 | OE1 | GLN | 1362 | -24.758 | 7.933 | 52.760 | 1.00 28.92 |
| ATOM | 9198 | NE2 | GLN | 1362 | -24.195 | 6.345 | 51.266 | 1.00 29.63 |
| ATOM | 9199 | С | GLN | 1362 | -24.439 | 3.519 | 54.194 | 1.00 23.54 |
| ATOM | 9200 | 0 | GLN | 1362 | -24.409 | 3.157 | 53.019 | 1.00 23.64 |
| ATOM | 9201 | N | LEU | 1363 | -23.984 | 2.764 | 55.190 | 1.00 24.10 |
| ATOM | 9202 | CA | LEU | 1363 | -23.418 | 1.441 | 54.932 | 1.00 25.78 |
| ATOM | 9203 | CB | LEU | 1363 | -22.840 | 0.831 | 56.214 | 1.00 27.37 |
| ATOM | 9204 | CG | LEU | 1363 | -21.488 | 1.337 | 56.715 | 1.00 30.02 |
| ATOM | 9205 | CD1 | LEU | 1363 | -21.078 | 0.539 | 57.948 | 1.00 29.46 |
| MOTA | 9206 | | LEU | 1363 | -20.436 | 1.184 | 55.628 | 1.00 30.43 |
| MOTA | 9207 | С | LEU | 1363 | -24.453 | 0.485 | 54.354 | 1.00 25.61 |
| ATOM | 9208 | 0 | LEU | 1363 | -24.186 | -0.215 | 53.378 | 1.00 24.86 |
| ATOM | 9209 | N | LEU | 1364 | -25.633 | 0.446 | 54.965 | 1.00 25.26 |
| ATOM | 9210 | CA | LEU | 1364 | -26.690 | -0.433 | 54.486 | 1.00 25.78 |
| MOTA | 9211 | СВ | LEU | 1364 | -27.940 | -0.270 | 55.355 | 1.00 28.25 |
| MOTA | 9212 | CG | LEU | 1364 | -28.877 | -1.483 | 55.466 | 1.00 30.43 |
| ATOM | 9213 | | LEU | 1364 | -29.981 | -1.183 | 56.470 | 1.00 33.01 |
| ATOM | 9214 | CD2 | LEU | 1364 | -29.468 -26.996 | -1.809 -0.081 | 54.117 53.030 | 1.00 31.42 1.00 24.42 |
| ATOM | 9215 | С | LEU | 1364 1364 | -27.124 | -0.963 | 52.180 | 1.00 24.42 |
| MOTA MOTA | 9216 9217 | O N | LEU SER | 1365 | -27.124 | 1.216 | 52.748 | 1.00 24.75 |
| ATOM | 9217 | CA | SER | 1365 | -27.372 | 1.696 | 51.399 | 1.00 24.23 |
| ATOM | 9219 | CB | SER | 1365 | -27.440 | 3.226 | 51.388 | 1.00 25.49 |
| ATOM | 9220 | OG | SER | 1365 | -27.711 | 3.713 | 50.085 | 1.00 20.43 |
| ATOM | 9221 | C | SER | 1365 | -26.288 | 1.225 | 50.436 | 1.00 20.66 |
| ATOM | 9222 | Ö | SER | 1365 | -26.581 | 0.731 | 49.343 | 1.00 17.79 |
| ATOM | 9223 | N | ASP | 1366 | -25.033 | 1.397 | 50.841 | 1.00 19.04 |
| ATOM | 9224 | CA | ASP | 1366 | -23.902 | 0.971 | 50.013 | 1.00 18.22 |
| ATOM | 9225 | СВ | ASP | 1366 | -22.564 | 1.389 | 50.645 | 1.00 19.61 |
| ATOM | 9226 | CG | ASP | 1366 | -22.294 | 2.890 | 50.553 | 1.00 20.96 |
| ATOM | 9227 | OD1 | ASP | 1366 | -22.831 | 3.569 | 49.652 | 1.00 20.14 |
| MOTA | 9228 | OD2 | ASP | 1366 | -21.508 | 3.393 | 51.384 | 1.00 19.72 |
| ATOM | 9229 | С | ASP | 1366 | -23.914 | -0.547 | 49.824 | 1.00 16.69 |
| ATOM | 9230 | 0 | ASP | 1366 | -23.643 | -1.040 | 48.728 | 1.00 18.02 |
| ATOM | 9231 | N | ALA | 1367 | -24.216 | -1.291 | 50.885 | 1.00 15.72 |
| MOTA | 9232 | CA | ALA | 1367 | -24.244 | -2.748 | 50.783 | 1.00 16.03 |
| ATOM | 9233 | CB | ALA | 1367 | -24.598 | -3.372 | 52.136 | 1.00 16.32 |
| MOTA | 9234 | С | ALA | 1367 | -25.245 | -3.181 | 49.717 | 1.00 17.08 |
| ATOM | 9235 | 0 | ALA | 1367 | -24.944 | -4.032 | 48.878 | 1.00 15.80 |
| ATOM | 9236 | N | LEU | 1368 | -26.436 | -2.588 | 49.745 | 1.00 16.63 |
| MOTA | 9237 | CA | LEU | 1368 | -27.473 | -2.902 | 48.759 | 1.00 15.83 |
| ATOM | 9238 | CB | LEU | 1368 | -28.775 | -2.201 | 49.131 | 1.00 17.90 |
| ATOM | 9239 | CG | LEU | 1368 | -29.457 | -2.782 | 50.363 | 1.00 18.04 |
| MOTA | 9240 | CD1 | | 1368 | -30.451 | -1.771 -4.097 | 50.910 49.992 | 1.00 22.56 1.00 18.80 |
| ATOM ATOM | 9241 9242 | CD2 C | LEU LEU | 1368 1368 | -30.137 -27.060 | -2.475 | 47.360 | 1.00 15.44 |
| | | 0 | | | -27.309 | -3.189 | 46.390 | 1.00 17.08 |
| ATOM ATOM | 9243 9244 | N | LEU ALA | 1368 1369 | -26.437 | -1.304 | 47.265 | 1.00 15.14 |
| ATOM | 9245 | CA | ALA | 1369 | -25.985 | -0.781 | 45.984 | 1.00 15.71 |
| ATOM | 9246 | CB | ALA | 1369 | -25.393 | 0.609 | 46.164 | 1.00 16.16 |
| ATOM | 9247 | c | ALA | 1369 | -24.948 | -1.714 | 45.372 | 1.00 15.06 |
| ATOM | 9248 | 0 | ALA | 1369 | -24.979 | -1.985 | 44.172 | 1.00 13.93 |
| MOTA | 9249 | N | LEU | 1370 | -24.025 | -2.201 | 46.196 | 1.00 15.56 |
| ATOM | 9250 | CA | LEU | 1370 | -22.990 | -3.106 | 45.702 | 1.00 15.57 |
| MOTA | 9251 | CB | LEU | 1370 | -21.962 | -3.389 | 46.805 | 1.00 17.04 |
| ATOM | 9252 | CG | LEU | 1370 | -21.115 | -2.176 | 47.231 | 1.00 17.64 |
| ATOM | 9253 | CD1 | LEU | 1370 | -20.257 | -2.520 | 48.450 | 1.00 14.36 |
| MOTA | 9254 | CD2 | LEU | 1370 | -20.236 | -1.745 | 46.077 | 1.00 17.55 |
| ATOM | 9255 | С | LEU | 1370 | -23.639 | -4.395 | 45.228 | 1.00 16.16 |
| MOTA | 9256 | 0 | LEU | 1370 | -23.306 | -4.917 | 44.160 | 1.00 14.48 |
| ATOM | 9257 | N | GLU | | -24.573 | -4.912 | 46.020 | 1.00 15.93 |
| ATOM | 9258 | CA | GLU | 1371 | -25.269 | -6.142 | 45.647 | 1.00 16.46 |
| MOTA | 9259 | CB | GLU | 1371 | -26.264 | -6.540 | 46.745 | 1.00 17.16 |
| MOTA | 9260 | CG | GLU | 1371 | -27.134 | -7.735 | 46.381 | 1.00 20.30 |
| MOTA | 9261 | CD | GLU | 1371 | -28.084 | -8.098 | 47.491 | 1.00 19.27 |
| ATOM | 9262 | | GLU | 1371 | -28.878 | -7.224 | 47.897 | 1.00 18.29 |
| MOTA | 9263 | OE2 | GLU | 1371 | -28.029 -26.007 | -9.248 -5.960 | 47.964 | 1.00 23.87 |
| ATOM | 9264 | ,C | GLU | 1371 | -26.007 -25.894 | -5.960 -6.789 | 44.319 43.409 | 1.00 16.54 1.00 16.17 |
| ATOM | 9265 | O N | GLU | 1371 | -25.894 -26.757 | -6.789 -4.869 | 43.409 | 1.00 16.17 |
| ATOM ATOM | 9266 | N CA | ALA ALA | 1372 1372 | -27.516 | -4.809 -4.601 | 42.987 | 1.00 16.00 |
| ATOM | 9267 9268 | CB | ALA | 1372 | -28.354 | -3.328 | 43.161 | 1.00 16.45 |
| FILOR | 3200 | CD | AUA | 13/2 | 20.334 | 5.520 | | 10.13 |

| ATOM | 9269 | С | ALA | 1372 | -26.585 | -4.460 | 41.790 | 1.00 16.56 |
|------|------|-----|-----|------|---------|--------------------|--------|------------|
| ATOM | 9270 | 0 | ALA | 1372 | -26.953 | -4.791 | 40.660 | 1.00 15.51 |
| MOTA | 9271 | N | ALA | 1373 | -25.377 | -3.961 | 42.044 | 1.00 14.61 |
| ATOM | 9272 | CA | ALA | 1373 | -24.382 | -3.758 | 40.987 | 1.00 14.87 |
| ATOM | 9273 | CB | ALA | 1373 | -23.253 | -2.858 | 41.507 | 1.00 15.59 |
| ATOM | 9274 | С | ALA | 1373 | -23.804 | -5.077 | 40.477 | 1.00 14.66 |
| ATOM | 9275 | 0 | ALA | 1373 | -23.232 | -5.133 | 39.386 | 1.00 15.82 |
| ATOM | 9276 | N | GLY | 1374 | -23.935 | -6.132 | 41.273 | 1.00 14.12 |
| ATOM | 9277 | CA | GLY | 1374 | -23.427 | -7.423 | 40.846 | 1.00 14.74 |
| ATOM | 9278 | С | GLY | 1374 | -22.460 | -8.120 | 41.789 | 1.00 15.58 |
| ATOM | 9279 | 0 | GLY | 1374 | -22.046 | -9.250 | 41.513 | 1.00 17.25 |
| ATOM | 9280 | N | ALA | 1375 | -22.081 | -7.468 | 42.888 | 1.00 15.59 |
| ATOM | 9281 | CA | ALA | 1375 | -21.167 | -8.098 | 43.847 | 1.00 15.31 |
| ATOM | 9282 | CB | ALA | 1375 | -20.901 | -7.167 | 45.031 | 1.00 12.55 |
| ATOM | 9283 | C | ALA | 1375 | -21.815 | -9.390 | 44.336 | 1.00 15.80 |
| ATOM | 9284 | ō | ALA | 1375 | -23.000 | -9.408 | 44.659 | 1.00 17.75 |
| ATOM | 9285 | N | GLN | 1376 | -21.041 | -10.469 | 44.393 | 1.00 16.08 |
| ATOM | 9286 | CA | GLN | 1376 | -21.584 | -11.756 | 44.825 | 1.00 16.60 |
| ATOM | 9287 | CB | GLN | 1376 | | -12.857 | 43.887 | 1.00 16.95 |
| ATOM | 9288 | CG | GLN | 1376 | -21.526 | | 42.441 | 1.00 22.74 |
| MOTA | 9289 | CD | GLN | 1376 | -20.999 | | 41.484 | 1.00 24.07 |
| ATOM | 9290 | OE1 | | 1376 | | -14.809 | 41.477 | 1.00 29.42 |
| ATOM | 9291 | NE2 | GLN | 1376 | | -13.281 | 40.665 | 1.00 27.21 |
| ATOM | 9292 | C | GLN | 1376 | -21.217 | -12.076 | 46.269 | 1.00 17.00 |
| ATOM | 9293 | 0 | GLN | 1376 | | -13.079 | 46.829 | 1.00 17.05 |
| | | | | | | -11.199 | 46.860 | 1.00 17.03 |
| ATOM | 9294 | N | LEU | 1377 | -20.411 | | 48.232 | |
| ATOM | 9295 | CA | LEU | 1377 | -19.958 | -11.337 -12.164 | | |
| MOTA | 9296 | CB | LEU | 1377 | | | 48.280 | 1.00 21.20 |
| ATOM | 9297 | CG | LEU | 1377 | | -13.672 | 48.435 | 1.00 22.45 |
| MOTA | 9298 | | LEU | 1377 | | -14.317 | 48.174 | 1.00 22.86 |
| MOTA | 9299 | | LEU | 1377 | -19.279 | -13.991 | 49.840 | 1.00 22.77 |
| ATOM | 9300 | С | LEU | 1377 | -19.674 | -9.964 | 48.807 | 1.00 15.17 |
| MOTA | 9301 | 0 | LEU | 1377 | -19.404 | -9.017 | 48.068 | 1.00 15.26 |
| MOTA | 9302 | N | LEU | 1378 | -19.734 | -9.856 | 50.129 | 1.00 15.03 |
| MOTA | 9303 | CA | LEU | 1378 | -19.445 | -8.588 | 50.792 | 1.00 15.26 |
| MOTA | 9304 | CB | LEU | 1378 | -20.750 | -7.840 | 51.099 | 1.00 15.07 |
| MOTA | 9305 | CG | LEU | 1378 | -20.584 | -6.620 | 52.011 | 1.00 15.89 |
| ATOM | 9306 | | LEU | 1378 | -19.891 | -5.491 | 51.246 | 1.00 17.24 |
| MOTA | 9307 | | LEU | 1378 | -21.961 | -6.154 | 52.507 | 1.00 19.57 |
| MOTA | 9308 | С | LEU | 1378 | -18.679 | -8.808 | 52.090 | 1.00 15.81 |
| ATOM | 9309 | 0 | LEU | 1378 | -19.048 | -9.656 | 52.900 | 1.00 16.07 |
| MOTA | 9310 | N | VAL | 1379 | -17.599 | -8.060 | 52.282 | 1.00 16.13 |
| MOTA | 9311 | CA | VAL | 1379 | -16.845 | -8.160 | 53.523 | 1.00 16.26 |
| ATOM | 9312 | CB | VAL | 1379 | -15.297 | -8.136 | 53.275 | 1.00 14.82 |
| MOTA | 9313 | CG1 | | 1379 | -14.567 | -7.886 | 54.588 | 1.00 14.92 |
| MOTA | 9314 | CG2 | VAL | 1379 | -14.830 | -9.493 | 52.691 | 1.00 13.84 |
| MOTA | 9315 | С | VAL | 1379 | -17.245 | -6.955 | 54.383 | 1.00 16.23 |
| ATOM | 9316 | О | VAL | 1379 | -17.366 | -5.838 | 53.876 | 1.00 14.40 |
| ATOM | 9317 | N | LEU | 1380 | -17.502 | -7.200 | 55.667 | 1.00 17.52 |
| ATOM | 9318 | CA | LEU | 1380 | -17.869 | -6.150 | 56.626 | 1.00 18.33 |
| ATOM | 9319 | CB | LEU | 1380 | -19.228 | -6.426 | 57.264 | 1.00 23.25 |
| ATOM | 9320 | CG | LEU | 1380 | -20.451 | -5.763 | 56.649 | 1.00 27.26 |
| ATOM | 9321 | | LEU | 1380 | -21.679 | -6.205 | 57.436 | 1.00 29.17 |
| MOTA | 9322 | | LEU | 1380 | -20.310 | -4.237 | 56.689 | 1.00 28.64 |
| MOTA | 9323 | С | LEU | 1380 | -16.820 | -6.151 | 57.729 | 1.00 17.93 |
| ATOM | 9324 | О | LEU | 1380 | -16.671 | -7.142 | 58.438 | 1.00 17.27 |
| ATOM | 9325 | N | GLU | 1381 | -16.126 | -5.032 | 57.901 | 1.00 18.24 |
| MOTA | 9326 | CA | GLU | 1381 | -15.058 | -4.951 | 58.890 | 1.00 18.15 |
| MOTA | 9327 | CB | GLU | 1381 | -13.735 | -4.706 | 58.154 | 1.00 19.99 |
| MOTA | 9328 | CG | GLU | 1381 | -12.535 | -4.399 | 59.042 | 1.00 19.58 |
| ATOM | 9329 | CD | GLU | 1381 | -11.214 | -4.485 | 58.288 | 1.00 21.41 |
| ATOM | 9330 | OE1 | GLU | 1381 | -11.236 | -4.456 | 57.042 | 1.00 20.29 |
| ATOM | 9331 | OE2 | GLU | 1381 | -10.152 | -4.579 | 58.939 | 1.00 22.00 |
| MOTA | 9332 | C | GLU | 1381 | -15.222 | -3.910 | 59.995 | 1.00 18.95 |
| MOTA | 9333 | 0 | GLU | 1381 | -15.451 | -2.733 | 59.725 | 1.00 17.56 |
| MOTA | 9334 | N | CYS | 1382 | -15.094 | -4.355 | 61.242 | 1.00 18.95 |
| MOTA | 9335 | CA | CYS | 1382 | -15.168 | -3.456 | 62.388 | 1.00 20.18 |
| MOTA | 9336 | CB | CYS | 1382 | -13.858 | -2.676 | 62.501 | 1.00 20.94 |
| MOTA | 9337 | SG | CYS | 1382 | -12.444 | -3.736 | 62.885 | 1.00 25.87 |
| MOTA | 9338 | С | CYS | 1382 | -16.344 | -2.488 | 62.383 | 1.00 19.45 |
| MOTA | 9339 | 0 | CYS | 1382 | -16.181 | -1.279 | 62.191 | 1.00 19.01 |
| ATOM | 9340 | N | VAL | 1383 | -17.523 | -3.038 | 62.631 | 1.00 20.89 |
| MOTA | 9341 | CA | VAL | 1383 | -18.753 | -2.272 | 62.665 | 1.00 21.85 |
| MOTA | 9342 | CB | VAL | 1383 | ~19.513 | -2.440 | 61.324 | 1.00 23.50 |
| MOTA | 9343 | CG1 | VAL | 1383 | -20.222 | -3.785 | 61.286 | 1.00 18.79 |
| MOTA | 9344 | CG2 | VAL | 1383 | -20.471 | -1.295 | 61.113 | 1.00 26.50 |
| MOTA | 9345 | C | VAL | 1383 | -19.576 | -2.863 | 63.809 | 1.00 22.30 |
| | | | | | | | | |

| ATOM 9346 O VAL 1383 -19.434 -4.042 64.131 1.00 22.63 ATOM 9348 CD PRO 1384 -20.747 -0.631 64.237 1.00 21.90 ATOM 9348 CD PRO 1384 -20.747 -0.631 64.237 1.00 21.90 ATOM 9350 CB PRO 1384 -22.131 -2.068 65.548 1.00 22.79 ATOM 9351 CG PRO 1384 -22.162 -0.556 64.737 1.00 26.47 ATOM 9351 CG PRO 1384 -22.162 -0.556 64.737 1.00 26.45 ATOM 9352 C PRO 1384 -22.162 -0.556 64.737 1.00 24.45 ATOM 9353 O PRO 1384 -22.200 -3.841 65.101 1.00 24.45 ATOM 9355 CA VAL 1385 -22.140 -4.808 66.003 1.00 24.71 ATOM 9355 CA VAL 1385 -22.866 -6.050 65.77 1.00 26.27 ATOM 9356 CB VAL 1385 -22.866 -6.050 65.77 1.00 26.27 ATOM 9357 CGI VAL 1385 -22.866 -6.050 65.77 1.00 27.89 ATOM 9358 CQ VAL 1385 -22.866 -6.050 65.77 1.00 27.89 ATOM 9356 CB VAL 1385 -22.866 -6.107 66.991 1.00 27.91 ATOM 9356 CB VAL 1385 -22.866 -6.107 66.991 1.00 27.91 ATOM 9360 O VAL 1385 -24.772 -6.513 64.366 1.00 27.91 ATOM 9361 N GLU 1386 -24.884 -4.734 65.367 1.00 27.92 ATOM 9362 CA GLU 1386 -26.241 -4.372 65.367 1.00 27.92 ATOM 9365 CB GLU 1386 -26.241 -4.372 65.367 1.00 27.92 ATOM 9366 CB GLU 1386 -26.241 -4.372 65.367 1.00 27.92 ATOM 9367 CE GLU 1386 -26.241 -4.372 65.367 1.00 27.93 ATOM 9367 CE GLU 1386 -26.241 -4.372 65.367 1.00 30.32 ATOM 9367 CE GLU 1386 -26.241 -4.372 65.367 1.00 30.32 ATOM 9367 CE GLU 1386 -27.157 -4.601 63.168 1.00 31.48 ATOM 9370 N LEU 1387 -22.590 -2.912 61.992 1.00 27.95 ATOM 9371 CA LEU 1387 -22.590 -2.912 61.992 1.00 27.95 ATOM 9377 CB LEU 1387 -22.590 -2.912 61.992 1.00 27.95 ATOM 9378 C LEU 1387 -22.590 -2.912 61.992 1.00 26.77 ATOM 9379 C A LAB 1388 -22.594 -2.993 6.800 1.00 27.80 ATOM 9379 C A LEU 1387 -22.590 -2.912 61.992 1.00 26.77 ATOM 9379 C A LEU 1387 -22.590 -2.912 61.992 1.00 26.77 ATOM 9379 C A LEU 1387 -22.590 -2.912 61.992 1.00 26.03 ATOM 9379 C A LEU 1387 -22.590 -2.912 61.992 1.00 26.03 ATOM 9398 C LEU 1387 -22.590 -2.912 61.992 1.00 26.03 ATOM 9398 C LEU 1387 -22.590 -2.912 61.992 1.00 26.03 ATOM 9398 C LEU 1388 -22.754 -1.993 61.00 26.60 ATOM 9398 C LEU 1388 -22.754 -1.993 61.00 26.00 ATOM 9398 C LEU 1387 -22.894 -2.9 | | | | | | | | | |
|--|------|------|-----|-----|------|---------|---------|--------|------------|
| ATOM 9347 N PRO 1384 -20.432 -2.050 64.454 1.00 22.70 ATOM 9349 CD PRO 1384 -21.231 -2.608 65.548 1.00 23.71 ATOM 9350 CB PRO 1384 -22.140 -1.441 65.952 1.00 24.77 ATOM 9351 CB PRO 1384 -22.140 -1.441 65.952 1.00 24.71 ATOM 9351 C PRO 1384 -22.162 -0.556 64.735 1.00 25.75 ATOM 9352 C PRO 1384 -22.099 -3.841 65.101 1.00 24.74 ATOM 9353 N PRO 1384 -22.099 -3.841 65.101 1.00 23.74 ATOM 9355 CA VAL 1385 -22.866 -6.050 65.727 1.00 25.23 ATOM 9355 CA VAL 1385 -22.866 -6.050 65.727 1.00 26.23 ATOM 9355 CA VAL 1385 -22.866 -6.050 65.727 1.00 26.23 ATOM 9355 CA VAL 1385 -22.866 -6.050 65.727 1.00 26.23 ATOM 9356 CB VAL 1385 -22.864 -6.050 65.727 1.00 27.76 ATOM 9356 CB VAL 1385 -22.864 -6.050 65.727 1.00 27.76 ATOM 9356 CQ VAL 1385 -22.864 -6.050 65.727 1.00 27.72 ATOM 9356 CQ VAL 1385 -24.626 -1.011 67.635 1.00 29.95 ATOM 9356 CQ VAL 1385 -24.626 -5.151 64.366 1.00 27.72 ATOM 9360 N VAL 1385 -24.626 -5.151 64.566 1.00 27.72 ATOM 9361 N VAL 1385 -24.626 -5.151 64.566 1.00 27.72 ATOM 9361 N VAL 1385 -24.626 -4.172 65.151 64.00 27.87 ATOM 9362 CA GLU 1386 -24.772 -6.151 65.51 61.00 29.95 ATOM 9366 CB CA GLU 1386 -26.241 -4.128 67.53 1.00 27.97 ATOM 9366 OB CLU 1386 -26.241 -4.128 67.53 1.00 27.84 ATOM 9367 OB CLU 1386 -27.084 -5.051 68.325 1.00 27.84 ATOM 9367 OB CLU 1386 -27.084 -5.051 68.325 1.00 27.84 ATOM 9369 N CE GLU 1386 -27.784 -5.051 68.325 1.00 27.84 ATOM 9370 N CE GLU 1386 -27.784 -5.051 68.325 1.00 27.85 ATOM 9371 CA LEU 1387 -22.535 3.271 60.128 1.00 27.85 ATOM 9371 CA LEU 1387 -22.590 -2.12 61.92 61.00 27.86 ATOM 9371 CA LEU 1387 -22.590 -2.12 61.92 61.00 27.86 ATOM 9371 CA LEU 1387 -22.590 -2.12 61.92 61.00 27.86 ATOM 9378 CD LEU 1387 -22.590 -2.12 61.92 61.00 27.86 ATOM 9378 CD LEU 1387 -22.294 0.148 60.577 1.00 27.95 ATOM 9378 CD LEU 1387 -22.590 -2.12 61.95 96.10 27.86 ATOM 9378 CD LEU 1387 -22.590 -2.12 61.95 96.10 0.2 7.86 ATOM 9378 CD LEU 1387 -22.590 -2.12 61.95 96.10 0.2 7.86 ATOM 9378 CD LEU 1387 -22.590 -2.12 61.95 96.10 0.2 7.86 ATOM 9378 CD LEU 1387 -22.596 -2.10 9.4 1.48 60.577 1.00 25.87 ATOM | АТОМ | 9346 | 0 | VAL | 1383 | -19.434 | -4.042 | 64.131 | 1.00 22.63 |
| ATOM 9348 CD PRO 1384 -20.747 -0.631 64.237 1.00 21.90 ATOM 9350 CB PRO 1384 -22.140 -1.441 65.952 1.00 24.27 ATOM 9351 CG PRO 1384 -22.162 -0.556 64.375 1.00 26.27 ATOM 9355 CG PRO 1384 -22.160 -1.556 64.375 1.00 26.27 ATOM 9355 CP PRO 1384 -22.070 -3.841 65.101 1.00 24.45 ATOM 9355 CP PRO 1384 -22.070 -3.841 65.101 1.00 24.45 ATOM 9355 CP AVAL 1385 -22.140 -4.808 66.003 1.00 24.71 ATOM 9355 CP AVAL 1385 -22.856 -6.050 65.77 1.00 26.27 ATOM 9357 CGI VAL 1385 -22.866 -6.050 65.77 1.00 26.27 ATOM 9358 CQ VAL 1385 -22.866 -6.050 65.77 1.00 27.89 ATOM 9359 C VAL 1385 -22.866 -6.050 65.77 1.00 27.89 ATOM 9350 C VAL 1385 -22.866 -6.075 66.991 1.00 27.89 ATOM 9358 CQ VAL 1385 -22.866 -6.076 66.991 1.00 27.89 ATOM 9358 CQ VAL 1385 -22.866 -6.076 66.991 1.00 27.91 ATOM 9360 O VAL 1385 -24.772 -6.513 64.366 1.00 27.26 ATOM 9361 N GLU 1386 -24.884 -4.74 65.764 1.00 27.81 ATOM 9363 CB GLU 1386 -26.241 -4.372 65.367 1.00 30.32 ATOM 9365 CD GLU 1386 -26.241 -4.372 65.367 1.00 30.34 ATOM 9366 OEI GLU 1386 -26.171 -3.129 66.333 1.00 31.48 ATOM 9366 OEI GLU 1386 -26.174 -3.199 66.305 1.00 37.44 ATOM 9367 OEZ GLU 1386 -26.894 -5.051 68.325 1.00 27.95 ATOM 9369 N LEU 1386 -26.291 -4.088 63.472 1.00 27.91 ATOM 9370 N LEU 1386 -22.894 -5.051 68.325 1.00 29.05 ATOM 9371 CD LEU 1386 -22.894 -5.051 68.325 1.00 29.05 ATOM 9373 CG LEU 1386 -24.894 -4.90 60.846 1.00 29.05 ATOM 9373 CG LEU 1386 -24.894 -4.90 60.846 1.00 29.05 ATOM 9375 CD LEU 1387 -24.897 -0.767 60.722 1.00 26.03 ATOM 9376 CD LEU 1387 -24.897 -0.767 60.722 1.00 31.48 ATOM 9377 CD LEU 1387 -24.897 -0.767 60.722 1.00 31.48 ATOM 9378 CD LEU 1387 -24.897 -0.767 60.722 1.00 31.48 ATOM 9378 CD LEU 1387 -22.894 -0.914 60.92 1.00 29.03 ATOM 9378 CD LEU 1387 -22.894 -0.914 60.00 29.38 ATOM 9378 CD LEU 1387 -22.896 -0.914 60.00 29.38 ATOM 9378 CD LEU 1387 -22.896 -0.914 60.00 29.18 ATOM 9380 CD LYS 1389 -27.773 -7.773 65.500 1.00 26.63 ATOM 9381 CD LYS 1389 -27.896 -7.992 60.846 1.00 29.36 ATOM 9398 CD LYS 1389 -27.896 -5.10 60.648 1.00 29.38 ATOM 9399 CD LYS 1389 -27.896 -5.10 60 | | | | | | | | | |
| ATOM 9349 CA PRO 1384 -21.231 -2.608 65.548 1.00 23.71 ATOM 9351 CB PRO 1384 -22.162 -0.556 64.735 1.00 26.55 ATOM 9352 C PRO 1384 -22.109 -3.841 65.101 1.00 23.74 ATOM 9355 CA VAL 1385 -22.140 -3.808 66.031 1.00 23.74 ATOM 9355 CA VAL 1385 -22.1804 -6.917 66.911 1.00 27.62 ATOM 9355 CG VAL 1385 -23.606 -6.917 66.931 1.00 27.97 ATOM 9355 CG VAL 1385 -23.606 -8.261 66.321 1.00 27.97 ATOM 9356 CG VAL 1385 -24.726 -6.513 64.366 1.00 27.76 ATOM 9362 CA GLU <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> | | | | | | | | | |
| ATOM 9350 CB PRO 1384 -22.160 -1.555 64.755 1.00 26.25 ATOM 9352 C PRO 1384 -22.109 -3.841 65.101 1.00 24.45 ATOM 9355 C PRO 1384 -22.109 -3.841 65.101 1.00 24.47 ATOM 9355 CA VAL 1385 -22.140 -4.808 66.003 1.00 24.71 ATOM 9356 CB VAL 1385 -22.894 -6.917 66.991 1.00 27.89 ATOM 9356 CB VAL 1385 -22.984 -6.917 66.991 1.00 27.89 ATOM 9358 CG VAL 1385 -21.626 -7.101 67.635 1.00 27.89 ATOM 9360 N LU 1386 -24.263 -5.133 64.366 1.00 27.91 ATOM 9362 CA GLU | | | | | | | | | |
| ATOM 9351 CG PRO 1384 -22.162 -0.556 64.735 1.00 26.55 ATOM 9353 C PRO 1384 -22.097 -3.841 63.961 1.00 23.74 ATOM 9355 C PRO 1384 -22.097 -3.841 63.961 1.00 23.74 ATOM 9356 CR VAL 1385 -22.160 6-0.50 65.727 1.00 26.23 ATOM 9356 CB VAL 1385 -22.160 6-0.917 60.991 1.00 27.89 ATOM 9357 CGI VAL 1385 -22.986 -6.917 66.991 1.00 27.89 ATOM 9358 CG2 VAL 1385 -22.866 -6.917 66.991 1.00 27.89 ATOM 9358 CG2 VAL 1385 -22.866 -6.917 66.991 1.00 27.89 ATOM 9359 C VAL 1385 -22.626 -7.101 67.055 1.00 27.95 ATOM 9359 C VAL 1385 -24.722 -6.513 64.366 1.00 27.26 ATOM 9360 C VAL 1385 -24.722 -6.513 64.366 1.00 27.26 ATOM 9361 N GUU 1386 -24.772 -6.513 64.366 1.00 27.26 ATOM 9362 CA GUU 1386 -26.241 -4.372 65.367 1.00 30.32 ATOM 9363 CB GUU 1386 -26.241 -4.372 65.367 1.00 30.32 ATOM 9365 CD GUU 1386 -26.182 -2.988 67.554 1.00 27.87 ATOM 9365 CD GUU 1386 -26.182 -2.988 67.554 1.00 27.87 ATOM 9365 CD GUU 1386 -26.182 -2.988 67.555 1.00 37.12 ATOM 9367 CP2 GUU 1386 -26.291 -4.399 68.280 1.00 39.44 ATOM 9366 CD GUU 1386 -26.291 -4.399 68.280 1.00 39.44 ATOM 9367 CP2 GUU 1386 -26.291 -4.088 63.872 1.00 29.04 ATOM 9367 CP2 GUU 1386 -22.984 -4.599 68.810 1.00 40.64 ATOM 9369 C GUU 1386 -22.994 -4.599 68.810 1.00 40.64 ATOM 9367 CP2 GUU 1386 -22.994 -4.599 68.810 1.00 29.05 ATOM 9371 CA LEUI 1387 -22.5353 -3.271 63.396 1.00 29.05 ATOM 9377 C LEUI 1387 -22.193 -1.870 61.794 1.00 29.05 ATOM 9377 C LEUI 1387 -22.193 -1.870 61.794 1.00 29.08 ATOM 9378 C LEUI 1387 -22.194 -1.896 1.00 29.08 ATOM 9375 C LEUI 1387 -22.194 -1.896 1.00 29.08 ATOM 9376 C LEUI 1387 -22.194 -1.996 1.00 20.29 ATOM 9377 C LEUI 1387 -22.194 -1.996 1.00 20.29 ATOM 9378 C LEUI 1387 -22.194 -1.996 1.00 20.29 ATOM 9378 C LEUI 1387 -22.194 -1.996 1.00 20.29 ATOM 9379 C LEUI 1387 -22.194 -1.996 1.00 20.29 ATOM 9379 C LEUI 1387 -22.194 -1.996 1.00 20.29 ATOM 9379 C LEUI 1387 -22.194 -1.996 1.00 20.29 ATOM 9379 C LEUI 1387 -22.194 -1.996 1.00 20.29 ATOM 9379 C LEUI 1387 -22.194 -1.996 1.00 20.29 ATOM 9380 C A ALA 1388 -22.966 -1.996 1.00 20.29 ATOM 9380 C A ALA 1388 -22.966 -1.99 | | | | | | | | | |
| ATOM 9352 C PRO 1384 -22.009 -3.841 65.101 1.00 24.45 ATOM 9358 N PRO 1384 -22.470 -3.914 63.061 1.00 23.74 ATOM 9355 C N VAL 1385 -22.410 -4.808 66.003 1.00 24.71 ATOM 9356 C N VAL 1385 -22.856 -6.050 65.727 1.00 26.23 ATOM 9357 COI VAL 1385 -22.856 -6.050 65.727 1.00 27.76 ATOM 9358 C CV VAL 1385 -22.856 -8.261 66.032 1.00 27.76 ATOM 9358 C CV VAL 1385 -22.856 -8.261 66.032 1.00 27.76 ATOM 9358 C CV VAL 1385 -22.856 -8.261 66.032 1.00 27.76 ATOM 9360 O VAL 1385 -21.626 -7.101 67.635 1.00 29.95 ATOM 9360 O VAL 1385 -24.263 5.783 65.219 1.00 27.91 ATOM 9360 O VAL 1385 -24.263 5.783 65.219 1.00 27.91 ATOM 9360 C VAL 1385 -24.263 5.783 65.219 1.00 27.87 ATOM 9362 CA GLU 1386 -26.321 -4.372 65.367 1.00 30.32 ATOM 9365 CC GLU 1386 -26.317 -3.129 66.133 1.00 30.34 ATOM 9365 CC GLU 1386 -26.717 -3.129 66.133 1.00 31.48 ATOM 9366 CD GLU 1386 -26.077 -4.309 68.280 1.00 37.12 ATOM 9367 DE GLU 1386 -26.077 -4.309 68.280 1.00 37.42 ATOM 9368 C G GLU 1386 -26.077 -4.309 68.280 1.00 39.44 ATOM 9368 C G GLU 1386 -22.914 -4.599 68.810 1.00 40.64 ATOM 9370 N LEU 1387 -22.934 -4.084 63.872 1.00 29.05 ATOM 9371 CA LEU 1387 -22.5390 -3.271 63.396 1.00 27.86 ATOM 9373 C G LEU 1387 -22.5390 -3.271 63.396 1.00 27.86 ATOM 9375 C C LEU 1387 -22.394 0.148 60.577 1.00 29.05 ATOM 9377 C LEU 1387 -22.394 0.148 60.577 1.00 29.38 ATOM 9378 N LEU 1387 -22.497 -0.767 60.722 1.00 31.48 ATOM 9378 N LAL 1388 -22.3758 6-1.99 60.464 1.00 29.38 ATOM 9378 C LEU 1387 -22.390 -4.484 61.281 1.00 26.22 ATOM 9378 N ALA 1388 -22.3758 -6.199 60.464 1.00 23.30 ATOM 9380 C B ALA 1388 -22.3758 -6.199 60.464 1.00 23.30 ATOM 9381 C ALA 1388 -22.3758 -6.199 60.464 1.00 23.30 ATOM 9381 C ALA 1388 -22.3758 -6.199 60.464 1.00 23.30 ATOM 9380 C B ALA 1388 -22.3758 -6.199 60.464 1.00 23.61 ATOM 9380 C B ALA 1388 -22.3758 -6.199 60.664 1.00 23.03 ATOM 9381 C AL XI 1389 -27.753 -7.694 62.992 1.00 23.03 ATOM 9380 C C B ALA 1388 -22.3758 -6.199 60.664 1.00 23.03 ATOM 9380 C C B ALA 1388 -22.3758 -6.199 60.654 1.00 23.63 ATOM 9391 C A ALA 1388 -22.3758 -6.199 60.654 1.00 | | | | | | | | | |
| ATOM | | | | | | | | | |
| ATOM 9354 N VAL 1385 -22.140 -4.808 66.003 1.00 24.71 ATOM 9355 C R VAL 1385 -22.886 -6.050 65.727 1.00 26.23 ATOM 9356 CR VAL 1385 -22.886 -6.050 65.727 1.00 27.86 ATOM 9357 CGI VAL 1385 -22.886 -6.951 66.991 1.00 27.86 ATOM 9358 CGZ VAL 1385 -22.866 -7.101 67.635 1.00 29.95 ATOM 9359 C VAL 1385 -24.263 5.783 65.219 1.00 27.76 ATOM 9360 O VAL 1385 -24.263 5.783 65.219 1.00 27.91 ATOM 9361 N GUI 1386 -24.281 -4.374 65.754 1.00 27.87 ATOM 9362 CA GUI 1386 -24.884 -4.734 65.754 1.00 30.32 ATOM 9363 CB GUI 1386 -26.217 -4.372 65.367 1.00 30.32 ATOM 9364 CG GUI 1386 -26.217 -4.329 65.633 1.00 37.12 ATOM 9365 CD GUI 1386 -26.717 -3.129 66.133 1.00 37.12 ATOM 9366 CDI GUI 1386 -26.077 -4.309 68.280 1.00 37.42 ATOM 9367 C VAL 1385 -24.284 -4.599 68.810 1.00 40.64 ATOM 9368 C GUI 1386 -26.291 -4.691 63.368 1.00 29.05 ATOM 9370 N LEU 1387 -25.239 -2.912 61.982 1.00 42.78 ATOM 9370 N LEU 1387 -25.239 -2.912 61.982 1.00 26.78 ATOM 9371 CB LEU 1387 -22.497 -0.767 60.722 1.00 31.48 ATOM 9372 CB LEU 1387 -24.997 -0.767 60.722 1.00 31.48 ATOM 9375 C D LEU 1387 -24.997 -0.767 60.722 1.00 31.48 ATOM 9376 C LEU 1387 -24.997 -0.767 60.722 1.00 31.48 ATOM 9377 CD LEU 1387 -24.997 -0.767 60.722 1.00 31.48 ATOM 9378 N LAL 1388 -22.394 -4.394 69.79 1.00 22.93 ATOM 9377 C LEU 1387 -24.997 -0.767 60.722 1.00 31.48 ATOM 9378 N LAL 1388 -22.394 -1.396 69.391 1.00 23.03 ATOM 9378 C LEU 1387 -24.997 -0.767 60.722 1.00 31.48 ATOM 9380 C LEU 1387 -24.997 -0.767 60.722 1.00 31.48 ATOM 9381 C LEU 1387 -24.997 -0.767 60.722 1.00 31.48 ATOM 9378 N LAL 1388 -22.396 -2.992 61.992 1.00 22.93 ATOM 9378 N LAL 1388 -22.396 -2.992 61.992 1.00 22.93 ATOM 9379 C A LAL 1388 -22.396 -1.396 60.079 1.00 24.73 ATOM 9380 C B ALA 1388 -22.396 -1.396 60.079 1.00 24.73 ATOM 9381 C LEU 1387 -24.997 -0.767 60.722 1.00 31.49 ATOM 9380 C B ALA 1388 -22.396 -1.396 60.079 1.00 24.73 ATOM 9381 C LEU 1387 -24.997 -0.767 60.722 1.00 31.04 ATOM 9381 C ALC 1388 -22.396 -2.391 60.099 1.00 24.74 ATOM 9389 N L LE 1389 -27.858 -6.199 60.846 1.00 23.03 ATOM 9380 C ALA 1388 -22.3 | | | | | | | | | |
| ATOM 9355 CA VAL 1385 -22.856 -6.050 65.727 1.00 26.23 ATOM 9357 CG1 VAL 1385 -22.984 6-6.917 60.991 1.00 27.89 ATOM 9358 CG2 VAL 1385 -22.966 -8.261 66.632 1.00 27.76 ATOM 9358 CG2 VAL 1385 -22.626 -7.101 67.635 1.00 27.95 ATOM 9359 C VAL 1385 -24.626 -7.101 67.635 1.00 27.95 ATOM 9360 C VAL 1385 -24.626 -5.783 65.219 1.00 27.95 ATOM 9361 N GUU 1386 -24.772 -6.513 64.366 1.00 27.26 ATOM 9361 N GUU 1386 -24.772 -6.513 64.366 1.00 27.26 ATOM 9362 CA GUU 1386 -26.241 -4.372 65.367 1.00 30.32 ATOM 9363 CB GUU 1386 -26.241 -4.372 65.367 1.00 30.32 ATOM 9365 CD GUU 1386 -26.242 -2.988 67.553 1.00 37.12 ATOM 9365 CD GUU 1386 -26.182 -2.988 67.553 1.00 37.12 ATOM 9365 CD GUU 1386 -26.182 -2.988 67.553 1.00 37.12 ATOM 9367 CD2 GUU 1386 -26.247 -4.309 68.280 1.00 39.44 ATOM 9366 CD GUU 1386 -26.291 -4.088 63.872 1.00 29.04 ATOM 9367 CD2 GUU 1386 -26.291 -4.088 63.872 1.00 29.04 ATOM 9367 CD2 GUU 1386 -22.994 -4.599 68.810 1.00 40.64 ATOM 9369 O GUU 1386 -22.994 -4.599 68.810 1.00 40.64 ATOM 9367 CD2 GUU 1386 -22.291 -4.088 63.872 1.00 29.04 ATOM 9370 N LEU 1387 -25.353 3.271 63.368 1.00 29.05 ATOM 9371 CA LEU 1387 -25.353 3.271 63.368 1.00 29.05 ATOM 9371 CA LEU 1387 -22.493 -1.870 61.740 1.00 29.38 ATOM 9374 CD LEU 1387 -22.493 -1.870 61.740 1.00 29.38 ATOM 9375 CD LEU 1387 -22.493 -1.870 61.740 1.00 29.38 ATOM 9378 C LEU 1387 -22.493 -1.870 61.750 1.00 29.59 ATOM 9378 N ALA 1388 -22.736 -7.022 61.651 1.00 20.29.59 ATOM 9378 N ALA 1388 -22.736 -7.024 61.652 1.00 23.61 ATOM 9380 C B ALA 1388 -22.736 -7.024 61.652 1.00 23.61 ATOM 9381 C LEU 1387 -25.019 -4.148 61.752 1.00 24.78 ATOM 9381 C LEU 1387 -25.019 -4.148 61.00 23.03 ATOM 9381 C LEU 1387 -24.895 61.795 60.00 40.40 40.99 ATOM 9381 C LEU 1387 -25.019 -4.148 61.00 23.61 ATOM 9381 C LEU 1387 -25.019 -4.148 61.00 23.61 ATOM 9381 C LEU 1387 -25.019 -4.148 61.00 23.61 ATOM 9381 C LEU 1387 -25.019 -4.148 61.00 23.61 ATOM 9381 C LEU 1387 -25.019 -4.148 61.00 23.61 ATOM 9381 C LEU 1388 -25.301 -7.024 61.625 1.00 23.63 ATOM 9381 C LEU 1388 -25.301 -7.024 61.625 1.00 23.63 A | | | | | | | | | |
| ATOM 9356 CB VAL 1385 -22.984 -6.917 66.991 1.00 27.86 ATOM 9357 CGI VAL 1385 -22.626 -7.101 67.635 1.00 29.95 ATOM 9358 CG2 VAL 1385 -21.626 -7.101 67.635 1.00 29.95 ATOM 9360 O VAL 1385 -24.727 -6.513 64.366 1.00 27.76 ATOM 9361 N GUI 1386 -24.263 -7.83 65.291 1.00 27.91 ATOM 9362 CA GUU 1386 -24.884 -4.734 65.754 1.00 30.32 ATOM 9363 CB GUI 1386 -26.241 -4.372 65.367 1.00 30.32 ATOM 9365 CD GUU 1386 -26.241 -4.372 65.367 1.00 30.32 ATOM 9365 CD GUU 1386 -26.241 -4.372 65.367 1.00 31.48 ATOM 9366 CEI GUU 1386 -26.241 -4.372 65.367 1.00 37.12 ATOM 9366 CEI GUU 1386 -26.077 -4.309 68.280 1.00 37.12 ATOM 9367 CD GUU 1386 -26.077 -4.309 68.280 1.00 37.42 ATOM 9368 C GUU 1386 -27.284 -5.951 68.325 1.00 37.42 ATOM 9368 C GUU 1386 -27.284 -5.959 68.810 1.00 42.32 ATOM 9370 N EU 1387 -26.297 -4.601 63.168 172 1.00 29.04 ATOM 9371 CD EU 1387 -25.353 -3.271 63.396 1.00 29.05 ATOM 9371 CB EUI 1387 -22.990 -2.912 61.982 1.00 26.77 ATOM 9373 CD EUI 1387 -22.990 -2.912 61.982 1.00 26.78 ATOM 9374 CD LEUI 1387 -24.997 -0.767 60.722 1.00 31.48 ATOM 9375 CD EUI 1387 -24.997 -0.767 60.722 1.00 31.48 ATOM 9376 C EUI 1387 -24.997 -0.767 60.722 1.00 31.48 ATOM 9377 CD LEUI 1387 -24.997 -0.767 60.722 1.00 31.48 ATOM 9378 N ALLA 1388 -23.558 -6.199 60.846 1.00 29.58 ATOM 9378 N ALLA 1388 -22.567 -4.338 60.079 1.00 24.83 ATOM 9378 C EL I387 -25.019 -4.188 61.128 1.00 23.03 ATOM 9378 C EL I387 -25.019 -7.148 61.022 1.00 23.03 ATOM 9378 N ALLA 1388 -22.736 -7.926 61.625 1.00 23.03 ATOM 9380 C E ALLA 1388 -22.736 -6.199 60.846 1.00 23.61 ATOM 9381 C ALLA 1388 -22.736 -6.199 60.846 1.00 23.63 ATOM 9381 C ALLA 1388 -22.736 -6.199 60.846 1.00 23.63 ATOM 9382 C ALLA 1388 -22.736 -7.022 61.652 1.00 31.02 ATOM 9380 C E ALLA 1388 -22.736 -7.022 61.652 1.00 31.03 ATOM 9381 C ALLA 1388 -22.736 -7.022 61.652 1.00 32.02 ATOM 9381 C ALLA 1388 -22.736 -7.022 61.652 1.00 23.03 ATOM 9381 C ALLA 1388 -22.736 -7.022 61.656 1.00 20.03 ATOM 9381 C ALLA 1388 -22.736 -7.022 61.656 1.00 20.03 ATOM 9381 C ALLA 1388 -22.736 -7.022 61.662 1.00 23.03 ATOM 9381 | | | | | | | | | |
| APTOM | | | | | | | | | |
| ATOM 9358 CC VAL 1385 -24.263 -5.783 65.219 1.00 29.95 ATOM 9360 O VAL 1385 -24.263 -5.783 65.219 1.00 27.96 ATOM 9361 N GLU 1386 -24.884 -4.734 65.754 1.00 27.26 ATOM 9362 CA GLU 1386 -24.884 -4.734 65.754 1.00 37.12 ATOM 9363 CB GLU 1386 -26.717 -3.129 65.367 1.00 31.48 ATOM 9364 CG GLU 1386 -26.271 -4.372 65.367 1.00 37.12 ATOM 9365 CD GLU 1386 -26.871 -4.099 66.820 1.00 37.12 ATOM 9365 CD GLU 1386 -26.871 -4.099 66.820 1.00 47.12 ATOM 9365 CD GLU 1386 -27.084 -5.051 68.325 1.00 47.12 ATOM 9367 OEZ GLU 1386 -27.084 -5.051 68.325 1.00 42.32 ATOM 9367 OEZ GLU 1386 -26.271 -4.389 68.810 1.00 42.32 ATOM 9369 O GLU 1386 -26.291 -4.088 63.792 1.00 29.05 ATOM 9370 N LEU 1387 -25.353 -3.271 63.396 1.00 27.86 ATOM 9371 CA LEU 1387 -25.353 -3.271 63.396 1.00 27.86 ATOM 9373 CG LEU 1387 -25.353 -3.271 61.396 1.00 27.86 ATOM 9373 CG LEU 1387 -24.193 -1.870 61.740 1.00 29.38 ATOM 9373 CG LEU 1387 -24.193 -1.870 61.740 1.00 29.38 ATOM 9373 CG LEU 1387 -24.193 -1.870 60.722 1.00 31.48 ATOM 9375 CD LEU 1387 -23.294 0.148 60.577 1.00 29.59 ATOM 9375 CD LEU 1387 -23.294 0.148 60.577 1.00 29.58 ATOM 9378 C LEU 1387 -25.053 -4.896 60.577 1.00 29.58 ATOM 9378 C LEU 1387 -25.053 -4.896 60.577 1.00 29.58 ATOM 9378 C LEU 1387 -25.059 -4.186 61.128 1.00 26.28 ATOM 9378 C LEU 1387 -25.059 -4.186 61.128 1.00 26.28 ATOM 9380 CB ALA 1388 -24.092 -4.992 61.572 1.00 24.83 ATOM 9381 C ALA 1388 -24.092 -4.992 61.572 1.00 24.83 ATOM 9381 C ALA 1388 -24.092 -4.992 61.572 1.00 24.83 ATOM 9383 N LYS 1389 -27.583 -7.694 61.575 1.00 24.83 ATOM 9383 N LYS 1389 -27.583 -7.694 61.575 1.00 24.83 ATOM 9385 CB LYS 1389 -27.783 -7.694 61.575 1.00 24.83 ATOM 9380 CB ALA 1388 -25.041 -7.022 61.625 1.00 21.94 ATOM 9381 C ALA 1388 -24.092 -7.597 -8.133 64.203 1.00 38.20 ATOM 9380 CB ALA 1388 -24.092 -7.597 -4.186 61.705 1.00 24.83 ATOM 9380 CB ALA 1389 -27.583 -7.694 61.575 1.00 24.83 ATOM 9380 CB ALA 1389 -27.583 -7.694 61.575 1.00 24.83 ATOM 9380 CB ALA 1389 -27.583 -7.694 61.575 1.00 24.83 ATOM 9380 CB ALA 1389 -27.583 -7.694 61.595 1.00 24.83 ATOM 9380 | | | | | | | | | |
| ATOM 9359 C VAL 1385 -24,772 -6,513 64,366 1,00 27,25 ATOM 9361 N GLU 1386 -24,772 -6,513 64,366 1,00 27,26 ATOM 9362 CA GLU 1386 -26,241 -4,372 65,367 1,00 37,12 ATOM 9363 CB GLU 1386 -26,241 -4,372 65,367 1,00 37,12 ATOM 9365 CB GLU 1386 -26,241 -4,372 66,133 1,00 31,48 ATOM 9365 CD GLU 1386 -26,6182 -2,986 68,325 1,00 39,44 ATOM 9366 CE GLU 1386 -26,077 -4,309 68,280 1,00 39,44 ATOM 9366 CE GLU 1386 -26,077 -4,501 68,325 1,00 40,64 ATOM 9368 C GLU 1386 -26,027 -4,501 68,325 1,00 39,44 ATOM 9369 O GLU 1386 -26,291 -4,088 63,872 1,00 29,04 ATOM 9370 N LEU 1387 -25,253 -3,271 63,168 1,00 29,05 ATOM 9371 CA LEU 1387 -25,253 -3,271 63,168 1,00 29,05 ATOM 9373 CG LEU 1387 -23,294 -0,767 60,722 1,00 29,78 ATOM 9373 CG LEU 1387 -24,497 -0,767 60,722 1,00 29,38 ATOM 9375 CD LEU 1387 -24,497 -0,767 60,722 1,00 24,74 ATOM 9376 C LEU 1387 -24,876 -1,369 59,391 1,00 30,44 ATOM 9379 CA LAU 1388 -24,082 -1,488 60,577 1,00 29,59 ATOM 9377 C LEU 1387 -24,876 -1,489 60,577 1,00 29,59 ATOM 9379 CA LAU 1388 -24,082 -4,982 61,572 1,00 24,74 ATOM 9380 CB LAU 1388 -22,736 -1,926 60,846 1,00 24,74 ATOM 9380 CB ALA 1388 -22,736 -7,022 61,625 1,00 24,74 ATOM 9381 C LAU 1388 -22,736 -7,022 61,625 1,00 24,74 ATOM 9381 C LAU 1388 -22,736 -7,022 61,625 1,00 24,74 ATOM 9381 C LAU 1388 -22,736 -7,022 61,625 1,00 24,74 ATOM 9381 C LAU 1388 -22,736 -7,022 61,625 1,00 24,74 ATOM 9383 C LYS 1389 -27,739 -7,757 66,130 1,00 24,83 ATOM 9385 CB LYS 1389 -27,739 -7,757 66,148 1,00 23,64 ATOM 9380 C LYS 1389 | ATOM | | | | | | | | |
| ATTOM 9360 O VAL 1385 -24,872 -6.513 64,366 1,00 27,26 ATTOM 9361 N GLU 1386 -24,884 -4,734 65,754 1,00 27,87 ATTOM 9362 CA GLU 1386 -26,171 -3,129 65,367 1,00 30,32 ATTOM 9364 CG GLU 1386 -26,717 -3,129 65,367 1,00 37,12 ATTOM 9365 CD GLU 1386 -26,717 -3,129 66,133 1,00 37,12 ATTOM 9366 CD GLU 1386 -26,717 -4,309 68,810 1,00 37,12 ATTOM 9366 CD GLU 1386 -27,084 -5,051 68,325 1,00 42,32 ATTOM 9366 CD GLU 1386 -26,291 -4,088 63,872 1,00 29,05 ATTOM 9367 OEZ GLU 1386 -26,291 -4,088 63,872 1,00 29,05 ATTOM 9370 N LEU 1387 -25,353 -3,271 63,396 1,00 27,86 ATTOM 9371 CA LEU 1387 -25,353 -3,271 61,982 1,00 26,77 ATTOM 9372 CB LEU 1387 -24,193 -1,870 61,740 1,00 29,38 ATTOM 9373 CG LEU 1387 -24,193 -1,870 61,740 1,00 29,38 ATTOM 9375 CD LEU 1387 -23,294 -1,488 60,577 1,00 29,58 ATTOM 9376 C LEU 1387 -23,294 -1,488 60,577 1,00 29,58 ATTOM 9377 CD LEU 1387 -25,013 -4,188 60,577 1,00 29,58 ATTOM 9377 C LEU 1387 -25,013 -4,188 60,577 1,00 29,58 ATTOM 9378 C LEU 1387 -25,013 -4,188 60,577 1,00 24,83 ATTOM 9378 C LEU 1387 -25,013 -4,188 61,128 1,00 26,28 ATTOM 9380 CB ALA 1388 -24,082 -4,982 61,572 1,00 24,83 ATTOM 9380 CB ALA 1388 -24,082 -4,982 61,572 1,00 24,83 ATTOM 9380 CB ALA 1388 -24,082 -7,022 61,625 1,00 24,83 ATTOM 9385 CB LYS 1389 -27,753 -7,694 61,575 1,00 24,83 ATTOM 9385 CB LYS 1389 -27,753 -7,634 61,575 1,00 24,83 ATTOM 9385 CB LYS 1389 -27,753 -7,694 61,575 1,00 24,83 ATTOM 9385 CB LYS 1389 -27,835 -7,694 61,575 1,00 24,83 ATTOM 9385 CB LYS 1389 -27,853 -7,694 61,575 1,00 24,83 | ATOM | | CG2 | VAL | | | | | |
| ATOM 9361 N GLU 1386 | ATOM | 9359 | С | VAL | 1385 | -24.263 | -5.783 | 65.219 | 1.00 27.91 |
| ATOM 9362 CA GLU 1386 -26.241 -4.372 65.367 1.00 30.32 ATOM 9363 CB GLU 1386 -26.717 -3.129 66.133 1.00 31.48 ATOM 9365 CD GLU 1386 -26.182 -2.988 67.553 1.00 37.12 ATOM 9366 CB LU 1386 -26.077 -4.309 68.280 1.00 37.12 ATOM 9366 CB LU 1386 -27.084 -5.951 68.252 1.00 42.32 ATOM 9367 OEZ GLU 1386 -26.291 -4.088 63.872 1.00 29.05 ATOM 9367 OEZ GLU 1386 -26.291 -4.088 63.872 1.00 29.05 ATOM 9370 N LEU 1387 -25.353 -3.271 63.396 1.00 27.86 ATOM 9370 N LEU 1387 -25.353 -3.271 63.396 1.00 27.86 ATOM 9370 N LEU 1387 -25.353 -3.271 61.396 1.00 27.86 ATOM 9371 CA LEU 1387 -25.535 -1.00 61.740 1.00 27.86 ATOM 9373 CB LEU 1387 -24.193 -1.870 61.740 1.00 27.86 ATOM 9373 CG LEU 1387 -24.193 -1.870 60.722 1.00 31.48 ATOM 9373 CD LEU 1387 -23.294 0.148 60.577 1.00 29.59 ATOM 9375 CD2 LEU 1387 -23.294 0.148 60.577 1.00 29.59 ATOM 9377 C LEU 1387 -23.294 0.148 60.577 1.00 29.59 ATOM 9378 N ALA 1388 -24.082 -4.982 61.572 1.00 24.74 ATOM 9379 CA ALA 1388 -22.758 -6.199 60.846 1.00 23.61 ATOM 9380 CB ALA 1388 -22.758 -6.199 60.846 1.00 23.61 ATOM 9381 C ALA 1388 -22.756 -7.00 66.48 1.00 23.03 ATOM 9381 C ALA 1388 -22.756 -7.00 66.48 1.00 23.03 ATOM 9381 C ALA 1388 -25.041 -7.002 66.648 1.00 23.03 ATOM 9381 C ALA 1388 -25.041 -7.002 66.648 1.00 23.03 ATOM 9385 CB LYS 1389 -27.853 -7.694 61.705 60.864 1.00 23.03 ATOM 9385 CB LYS 1389 -27.853 -7.694 61.705 61.705 1.00 24.87 ATOM 9387 CG ARG 1390 -27.87 ATOM 9387 CB ARG 1390 -27.87 ATOM 9388 CB LYS 1389 -27.858 -7.894 61.656 1.00 27.87 ATOM 9387 CB ARG 1390 -28.866 -8.255 66.710 1.00 25.62 ATOM 9399 NZ LYS 1389 -27.895 -7.895 66.710 1.00 25.62 ATOM 9399 NZ LYS 1389 -27.896 -8.255 66.710 1.00 25.62 ATOM 9399 NZ LYS 1389 -27.896 -8.255 66.710 1.00 25.62 ATOM 9399 NZ LYS 1389 -27.896 -8.255 66.710 1.00 25.62 ATOM 9399 NZ LYS 1389 -27.896 -8.255 66.710 1.00 25.62 ATOM 9400 NZ LEE 1391 -25.248 -5.905 65.51 1.00 25.62 ATOM 9400 NZ LEE 1391 -25.248 - | MOTA | 9360 | 0 | VAL | 1385 | -24.772 | -6.513 | 64.366 | 1.00 27.26 |
| ATOM 9363 CB GLU 1386 -26.717 -3.129 66.133 1.00 31.48 ATOM 9365 CD GLU 1386 -26.182 -2.988 67.553 1.00 37.128 ATOM 9365 CD GLU 1386 -26.077 -4.309 68.280 1.00 39.44 ATOM 9366 OEI GLU 1386 -27.084 -5.051 68.325 1.00 42.32 ATOM 9367 OE2 GLU 1386 -24.984 -4.599 68.810 1.00 40.64 ATOM 9368 C GLU 1386 -24.984 -4.599 68.810 1.00 40.64 ATOM 9369 O GLU 1386 -27.157 -4.601 63.168 1.00 29.05 ATOM 9370 N LEU 1387 -25.235 -3.271 63.168 1.00 29.05 ATOM 9371 CA LEU 1387 -25.239 -2.912 61.982 1.00 27.86 ATOM 9373 CG LEU 1387 -25.299 -2.912 61.982 1.00 27.86 ATOM 9373 CG LEU 1387 -24.497 -0.767 60.722 1.00 27.86 ATOM 9373 CG LEU 1387 -24.497 -0.767 60.722 1.00 27.86 ATOM 9375 CD LEU 1387 -24.497 -0.767 60.722 1.00 31.48 ATOM 9375 CD LEU 1387 -24.497 -0.767 60.722 1.00 31.48 ATOM 9375 CD LEU 1387 -24.497 -0.767 60.722 1.00 31.48 ATOM 9376 C LEU 1387 -24.497 -0.767 60.722 1.00 31.48 ATOM 9378 N ALA 1388 -24.497 -0.767 60.722 1.00 24.74 ATOM 9378 N ALA 1388 -24.082 -4.982 61.572 1.00 24.74 ATOM 9379 CA ALA 1388 -25.301 -4.386 60.079 1.00 24.83 ATOM 9379 CA ALA 1388 -22.758 -6.199 60.846 1.00 23.61 ATOM 9381 C ALA 1388 -22.758 -6.199 60.846 1.00 23.61 ATOM 9381 C ALA 1388 -22.758 -6.199 60.846 1.00 23.61 ATOM 9382 O ALA 1388 -25.301 -7.517 95.960 1.00 24.34 ATOM 9382 O ALA 1388 -25.301 -7.517 95.960 1.00 24.34 ATOM 9385 CB LYS 1389 -27.114 -7.824 61.556 1.00 23.12 ATOM 9386 CG LYS 1389 -27.114 -7.824 61.556 1.00 23.12 ATOM 9387 CD LYS 1389 -27.114 -7.824 61.056 1.00 2.33 ATOM 9389 CC LYS 1389 -27.173 -7.773 65.500 1.00 23.03 ATOM 9389 CC LYS 1389 -27.174 -7.824 61.556 1.00 23.63 ATOM 9393 CA ARG 1390 -28.846 -3.904 59.910 1.00 42.83 ATOM 9393 CA ARG 1390 -28.846 -3.904 59.910 1.00 42.83 ATOM 9393 CA ARG 1390 -28.860 -5.916 60.564 1.00 23.68 ATOM 9393 CA ARG 1390 -28.980 -5.216 60.564 1.00 23.68 ATOM 9393 CA ARG 1390 -28.980 -5.216 60.564 1.00 23.68 ATOM 9393 CA ARG 1390 -28.980 -5.216 60.565 1.00 23.83 ATOM 9393 CA ARG 1390 -29.990 -7.525 60.566 1.00 23.83 ATOM 9400 CL ARG 1391 -22.291 -22.991 -22.991 1.00 23.83 ATOM 9400 CD ARG | ATOM | 9361 | N | GLU | 1386 | -24.884 | -4.734 | 65.754 | 1.00 27.87 |
| ATOM 9364 CG GLU 1386 -26.017 -4.309 68.280 1.00 37.12 ATOM 9365 CD GLU 1386 -26.077 -4.309 68.280 1.00 37.12 ATOM 9366 OEI GLU 1386 -26.077 -4.309 68.280 1.00 39.42 ATOM 9368 C GLU 1386 -27.157 -4.081 63.255 1.00 29.04 ATOM 9368 C GLU 1386 -27.157 -4.601 63.168 1.00 29.05 ATOM 9370 N LEU 1387 -25.353 -3.271 63.396 1.00 29.05 ATOM 9371 CA LEU 1387 -25.290 -2.912 61.982 1.00 26.77 ATOM 9372 CB LEU 1387 -22.393 -3.271 63.396 1.00 27.86 ATOM 9373 CG LEU 1387 -24.193 -1.870 61.740 1.00 29.35 ATOM 9373 CG LEU 1387 -24.497 -0.767 60.722 1.00 31.48 ATOM 9375 CD2 LEU 1387 -24.497 -0.767 60.722 1.00 31.48 ATOM 9376 C LEU 1387 -22.890 -1.369 59.391 1.00 33.03 ATOM 9377 O LEU 1387 -22.637 -4.338 60.079 1.00 24.83 ATOM 9378 N ALA 1388 -25.637 -4.338 60.079 1.00 24.83 ATOM 9379 CA ALA 1388 -22.736 7-0.22 61.625 1.00 24.74 ATOM 9380 CB ALA 1388 -22.736 7-0.22 61.625 1.00 24.74 ATOM 9381 C ALA 1388 -22.736 7-0.22 61.625 1.00 24.74 ATOM 9383 N LYS 1389 -25.844 -7.096 61.760 1.00 23.33 ATOM 9384 CA LYS 1389 -27.114 -7.824 61.526 1.00 22.34 ATOM 9386 CG LYS 1389 -27.134 -7.824 61.656 1.00 23.83 ATOM 9387 CD XS 1389 -27.134 -7.824 61.656 1.00 23.87 ATOM 9388 CE LYS 1389 -27.135 -7.624 61.656 1.00 27.87 ATOM 9389 NL 1388 -22.736 -7.622 61.655 1.00 21.94 ATOM 9380 CB ALA 1388 -22.736 -7.022 61.655 1.00 21.94 ATOM 9380 CB ALA 1388 -22.736 -7.022 61.656 1.00 26.664 ATOM 9380 CB ALA 1388 -22.736 -7.022 61.656 1.00 26.664 ATOM 9390 C LYS 1389 -27.737 -7.737 59.560 1.00 21.94 ATOM 9391 C ALA 1388 -22.736 -7.022 61.655 1.00 21.94 ATOM 9398 NL 1389 -27.737 -7.737 59.560 1.00 21.94 ATOM 9399 C A ARG 1390 -28.860 -5.516 59.960 1.00 21.80 ATOM 9391 C A ARG 1390 -28.860 -5.216 59.960 1.00 22.80 ATOM 9393 CA ARG 1390 -28.860 -5.546 59.769 1.00 33.40 ATOM 9393 CA ARG 1390 -28.860 -5.216 59.608 1.00 23.81 ATOM 9394 CB ARG 1390 -28.860 -5.216 59.608 1.00 23.81 ATOM 9404 CA ILE 1391 -22.2373 -7.383 55.001 0.00 24.87 ATOM 9407 CG ILE 1391 -22.6570 -8.653 56.657 1.00 23.92 ATOM 9408 CD ILE 1391 -22.6570 -8.053 57.003 1.00 23.81 ATOM 9408 CD ILE 1391 | ATOM | 9362 | CA | GLU | 1386 | -26.241 | -4.372 | 65.367 | 1.00 30.32 |
| ATOM 9364 CG GLU 1386 -26.017 -4.309 68.280 1.00 37.12 ATOM 9365 CD GLU 1386 -26.077 -4.309 68.280 1.00 37.12 ATOM 9366 OEI GLU 1386 -26.077 -4.309 68.280 1.00 39.42 ATOM 9368 C GLU 1386 -27.157 -4.081 63.255 1.00 29.04 ATOM 9368 C GLU 1386 -27.157 -4.601 63.168 1.00 29.05 ATOM 9370 N LEU 1387 -25.353 -3.271 63.396 1.00 29.05 ATOM 9371 CA LEU 1387 -25.290 -2.912 61.982 1.00 26.77 ATOM 9372 CB LEU 1387 -22.393 -3.271 63.396 1.00 27.86 ATOM 9373 CG LEU 1387 -24.193 -1.870 61.740 1.00 29.35 ATOM 9373 CG LEU 1387 -24.497 -0.767 60.722 1.00 31.48 ATOM 9375 CD2 LEU 1387 -24.497 -0.767 60.722 1.00 31.48 ATOM 9376 C LEU 1387 -22.890 -1.369 59.391 1.00 33.03 ATOM 9377 O LEU 1387 -22.637 -4.338 60.079 1.00 24.83 ATOM 9378 N ALA 1388 -25.637 -4.338 60.079 1.00 24.83 ATOM 9379 CA ALA 1388 -22.736 7-0.22 61.625 1.00 24.74 ATOM 9380 CB ALA 1388 -22.736 7-0.22 61.625 1.00 24.74 ATOM 9381 C ALA 1388 -22.736 7-0.22 61.625 1.00 24.74 ATOM 9383 N LYS 1389 -25.844 -7.096 61.760 1.00 23.33 ATOM 9384 CA LYS 1389 -27.114 -7.824 61.526 1.00 22.34 ATOM 9386 CG LYS 1389 -27.134 -7.824 61.656 1.00 23.83 ATOM 9387 CD XS 1389 -27.134 -7.824 61.656 1.00 23.87 ATOM 9388 CE LYS 1389 -27.135 -7.624 61.656 1.00 27.87 ATOM 9389 NL 1388 -22.736 -7.622 61.655 1.00 21.94 ATOM 9380 CB ALA 1388 -22.736 -7.022 61.655 1.00 21.94 ATOM 9380 CB ALA 1388 -22.736 -7.022 61.656 1.00 26.664 ATOM 9380 CB ALA 1388 -22.736 -7.022 61.656 1.00 26.664 ATOM 9390 C LYS 1389 -27.737 -7.737 59.560 1.00 21.94 ATOM 9391 C ALA 1388 -22.736 -7.022 61.655 1.00 21.94 ATOM 9398 NL 1389 -27.737 -7.737 59.560 1.00 21.94 ATOM 9399 C A ARG 1390 -28.860 -5.516 59.960 1.00 21.80 ATOM 9391 C A ARG 1390 -28.860 -5.216 59.960 1.00 22.80 ATOM 9393 CA ARG 1390 -28.860 -5.546 59.769 1.00 33.40 ATOM 9393 CA ARG 1390 -28.860 -5.216 59.608 1.00 23.81 ATOM 9394 CB ARG 1390 -28.860 -5.216 59.608 1.00 23.81 ATOM 9404 CA ILE 1391 -22.2373 -7.383 55.001 0.00 24.87 ATOM 9407 CG ILE 1391 -22.6570 -8.653 56.657 1.00 23.92 ATOM 9408 CD ILE 1391 -22.6570 -8.053 57.003 1.00 23.81 ATOM 9408 CD ILE 1391 | MOTA | 9363 | CB | GLU | 1386 | -26.717 | -3.129 | 66.133 | 1.00 31.48 |
| ATOM 9365 CD GLU 1386 -22-0.084 -5.051 68.325 1.00 42.32 ATOM 9367 OE2 GLU 1386 -27-0.84 -5.051 68.325 1.00 42.32 ATOM 9368 C GLU 1386 -24.994 -4.599 68.810 1.00 40.64 ATOM 9368 C GLU 1386 -22-1.57 -4.601 63.168 1.00 29.05 ATOM 9370 N LEU 1387 -25.333 -3.271 63.396 1.00 27.86 ATOM 9371 CA LEU 1387 -25.339 -3.271 61.93 1.00 27.86 ATOM 9372 CB LEU 1387 -22.390 -2.912 61.982 1.00 26.73 ATOM 9373 CG LEU 1387 -24.193 -1.870 61.740 1.00 29.38 ATOM 9374 CD1 LEU 1387 -24.193 -1.870 61.740 1.00 29.38 ATOM 9375 CD LEU 1387 -24.193 -1.870 61.740 1.00 29.59 ATOM 9376 C LEU 1387 -25.539 -9.912 61.982 1.00 10.00 20.33 ATOM 9376 C LEU 1387 -24.497 -0.767 60.722 1.00 31.46 ATOM 9377 O LEU 1387 -25.637 -4.338 60.079 1.00 24.83 ATOM 9378 N ALA 1388 -22.039 -4.148 61.128 1.00 26.22 ATOM 9379 CA ALA 1388 -22.039 -4.148 61.128 1.00 26.22 ATOM 9380 CB ALA 1388 -22.736 -6.199 60.846 1.00 23.61 ATOM 9381 C ALA 1388 -22.736 -7.022 61.625 1.00 21.43 ATOM 9383 N LYS 1389 -22.501 -7.517 59.560 1.00 23.83 ATOM 9383 N LYS 1389 -22.5844 -7.096 61.705 1.00 23.83 ATOM 9385 CB LYS 1389 -27.853 -7.694 62.992 1.00 32.83 ATOM 9386 CB LYS 1389 -27.853 -7.694 62.992 1.00 32.83 ATOM 9387 CD LYS 1389 -27.785 -7.694 62.992 1.00 32.12 ATOM 9388 CE LYS 1389 -27.785 -7.694 62.992 1.00 38.20 ATOM 9388 CB LYS 1389 -27.785 -7.694 62.992 1.00 28.43 ATOM 9389 NZ LYS 1389 -27.785 -7.694 62.992 1.00 28.43 ATOM 9390 C LYS 1389 -27.785 -7.694 62.992 1.00 28.43 ATOM 9391 C LYS 1389 -27.785 -7.694 62.992 1.00 28.43 ATOM 9398 NZ LYS 1389 -27.857 -7.694 62.992 1.00 28.43 ATOM 9398 NZ LYS 1389 -27.857 -7.694 62.992 1.00 28.43 ATOM 9390 C LYS 1389 -27.858 -7.817 67.999 1.00 44.93 ATOM 9391 C LYS 1389 -27.858 -7.817 67.999 1.00 43.94 ATOM 9391 C LYS 1389 -27.858 -7.817 67.999 1.00 43.94 ATOM 9390 C LYS 1389 -27.858 -7.817 67.999 1.00 43.93 ATOM 9391 C LYS 1389 -27.858 -7.817 67.999 1.00 43.93 ATOM 9394 CB ARG 1390 -28.866 -3.704 59.800 1.00 28.85 ATOM 9397 CB ARG 1390 -28.866 -3.704 59.800 1.00 28.85 ATOM 9401 C ARG 1390 -29.866 -3.704 59.800 1.00 28.85 ATOM 9402 C ARG 1 | | | CG | | 1386 | -26.182 | -2.988 | | 1.00 37.12 |
| ATOM 9366 OEI GLU 1386 -24.984 -4.599 68.810 1.00 42.32 ATOM 9368 C GLU 1386 -24.984 -4.599 68.810 1.00 40.64 ATOM 9368 C GLU 1386 -24.291 -4.088 63.872 1.00 29.04 ATOM 9370 N LEU 1387 -25.353 -3.271 63.396 1.00 27.86 ATOM 9371 CA LEU 1387 -25.230 -3.271 63.396 1.00 27.86 ATOM 9372 CB LEU 1387 -22.390 -1.870 61.740 1.00 29.05 ATOM 9373 CG LEU 1387 -24.497 -0.767 61.740 1.00 29.35 ATOM 9373 CG LEU 1387 -24.497 -0.767 61.740 1.00 29.35 ATOM 9375 CD2 LEU 1387 -24.497 -0.767 61.740 1.00 29.35 ATOM 9376 CL LEU 1387 -22.497 -0.767 66.722 1.00 31.48 ATOM 9376 C LEU 1387 -22.497 -0.767 60.722 1.00 31.48 ATOM 9377 O LEU 1387 -22.894 0.148 60.577 1.00 29.83 ATOM 9378 N ALA 1388 -24.876 -1.369 59.391 1.00 23.61 ATOM 9378 N ALA 1388 -22.5637 -4.338 60.079 1.00 24.83 ATOM 9378 N ALA 1388 -22.5637 -4.338 60.079 1.00 24.83 ATOM 9380 CB ALA 1388 -22.736 -7.022 61.625 1.00 24.74 ATOM 9381 C ALA 1388 -22.736 -7.022 61.625 1.00 24.74 ATOM 9382 O ALA 1388 -22.736 -7.022 61.625 1.00 21.94 ATOM 9383 N LYS 1389 -22.736 -7.022 61.655 1.00 21.94 ATOM 9384 CA LYS 1389 -27.114 -7.824 61.556 1.00 20.30 ATOM 9385 CB LYS 1389 -27.114 -7.824 61.656 1.00 23.87 ATOM 9386 CG LYS 1389 -27.114 -7.824 61.656 1.00 27.87 ATOM 9387 CL XIS 1389 -27.114 -7.824 61.656 1.00 27.87 ATOM 9388 CE LYS 1389 -27.114 -7.824 61.656 1.00 27.87 ATOM 9389 CA ARC 1390 -27.858 -7.694 62.992 1.00 32.12 ATOM 9390 C LYS 1389 -27.758 -7.617 67.999 1.00 44.99 ATOM 9391 C ARC 1389 -27.758 -7.817 67.999 1.00 44.99 ATOM 9393 CA ARC 1390 -28.860 -5.216 59.608 1.00 26.66 ATOM 9393 CA ARC 1390 -28.860 -5.216 59.608 1.00 26.86 ATOM 9393 CA ARC 1390 -28.860 -5.216 59.608 1.00 26.86 ATOM 9394 CB ARC 1390 -28.860 -5.216 59.608 1.00 26.86 ATOM 9395 CG ARC 1390 -28.860 -5.541 58.15 51.00 23.93 ATOM 9396 CD ARC 1390 -28.860 -5.545 56.670 1.00 23.53 ATOM 9400 CA RC 1391 -22.9394 -7.525 61.284 1.00 33.48 ATOM 9400 CA RC 1390 -28.866 -5.541 58.10 03.316 ATOM 9401 CA RC 1391 -22.2665 -5.663 56.700 1.00 22.88 ATOM 9402 CA RC 1391 -22.665 -5.663 56.670 1.00 22.88 ATOM 9404 CA ILE 1391 -22.66 | | 9365 | CD | GLU | 1386 | -26.077 | -4.309 | 68.280 | 1.00 39.44 |
| ATOM 9368 C | | | | | | | | | |
| ATOM 9368 C GLU 1386 -22.157 -4.088 63.872 1.00 29.04 ATOM 9370 N LEU 1387 -25.353 -3.271 63.396 1.00 29.08 ATOM 9371 CA LEU 1387 -25.353 -3.271 63.396 1.00 27.86 ATOM 9372 CB LEU 1387 -22.290 -1.870 61.740 1.00 29.38 ATOM 9373 CG LEU 1387 -24.497 -0.767 60.722 1.00 31.48 ATOM 9374 CDL LEU 1387 -22.4497 -0.767 60.722 1.00 31.48 ATOM 9375 CD2 LEU 1387 -22.4876 -1.369 59.391 1.00 33.03 ATOM 9376 C LEU 1387 -22.4876 -1.369 59.391 1.00 33.03 ATOM 9377 O LEU 1387 -25.637 -4.338 60.079 1.00 24.83 ATOM 9378 N ALA 1388 -25.637 -4.338 60.079 1.00 24.74 ATOM 9381 C ALA 1388 -22.736 -7.022 61.625 1.00 24.74 ATOM 9380 CB ALA 1388 -22.736 -7.022 61.625 1.00 24.74 ATOM 9381 C ALA 1388 -22.736 -7.022 61.625 1.00 21.94 ATOM 9383 N LYS 1389 -25.844 -7.096 61.760 1.00 20.30 ATOM 9384 CA LYS 1389 -27.853 -7.694 62.992 1.00 22.30 ATOM 9385 CB LYS 1389 -27.853 -7.694 62.992 1.00 22.30 ATOM 9386 CG LYS 1389 -27.853 -7.694 62.992 1.00 22.30 ATOM 9387 CD LYS 1389 -27.773 -7.694 62.992 1.00 22.32 ATOM 9388 CE LYS 1389 -27.783 -7.694 62.992 1.00 22.30 ATOM 9389 NZ LYS 1389 -27.853 -7.694 62.992 1.00 22.30 ATOM 9380 CB LYS 1389 -27.853 -7.694 62.992 1.00 22.30 ATOM 9387 CD LYS 1389 -27.783 -6.996 -8.255 66.710 1.00 44.69 ATOM 9398 CZ LYS 1389 -27.773 -7.73 64.203 1.00 32.12 ATOM 9398 CZ LYS 1389 -27.773 -7.73 64.203 1.00 32.12 ATOM 9399 CA LYS 1389 -27.773 -7.73 64.203 1.00 32.12 ATOM 9391 CD LYS 1389 -27.773 -7.694 62.992 1.00 32.12 ATOM 9391 CD LYS 1389 -27.793 -7.694 62.992 1.00 32.12 ATOM 9391 CD LYS 1389 -27.793 -7.694 62.992 1.00 32.12 ATOM 9391 CD LYS 1389 -27.793 -7.694 62.992 1.00 32.12 ATOM 9391 CD LYS 1389 -27.793 -7.694 62.992 1.00 32.12 ATOM 9391 CD LYS 1389 -27.793 -7.694 62.992 1.00 32.12 ATOM 9391 CD LYS 1389 -27.793 -7.694 62.992 1.00 32.12 ATOM 9391 CD LYS 1389 -27.793 -7.694 62.992 1.00 32.12 ATOM 9391 CD LYS 1389 -27.793 -7.694 62.992 1.00 32.12 ATOM 9391 CD LYS 1389 -27.696 -8.255 66.710 1.00 42.99 ATOM 9392 CD LYS 1389 -27.696 -8.255 66.710 1.00 42.99 ATOM 9400 CD ARC 1390 -28.996 -5.216 59.606 1.00 26.86 ATOM 9400 | | | | | | | | | |
| ATOM 9369 O GLU 1386 -27.157 -4.601 63.168 1.00 29.05 ATOM 9370 N LEU 1387 -25.353 -3.271 63.396 1.00 27.86 ATOM 9371 CA LEU 1387 -25.290 -2.912 61.396 1.00 26.77 ATOM 9373 CG LEU 1387 -24.193 -1.870 61.740 1.00 29.38 ATOM 9373 CG LEU 1387 -24.193 -1.870 61.740 1.00 29.38 ATOM 9374 CD1 LEU 1387 -24.497 -0.767 60.722 1.00 31.48 ATOM 9375 CD2 LEU 1387 -24.497 -0.767 60.722 1.00 31.48 ATOM 9376 C LEU 1387 -24.497 -0.767 60.722 1.00 31.48 ATOM 9375 CD2 LEU 1387 -24.876 -1.369 59.391 1.00 33.03 ATOM 9376 C LEU 1387 -25.637 -4.338 60.079 1.00 24.28 ATOM 9377 O LEU 1387 -25.637 -4.338 60.079 1.00 24.28 ATOM 9378 N ALA 1388 -24.082 -4.982 61.572 1.00 24.74 ATOM 9379 CA ALA 1388 -22.736 -7.022 61.625 1.00 24.74 ATOM 9380 CB ALA 1388 -22.736 -7.022 61.625 1.00 24.74 ATOM 9381 C ALA 1388 -25.041 -7.002 60.648 1.00 23.61 ATOM 9383 N LYS 1389 -25.844 -7.096 61.705 1.00 25.43 ATOM 9384 CA LYS 1389 -25.844 -7.096 61.705 1.00 25.43 ATOM 9386 CB LYS 1389 -27.114 -7.824 61.556 1.00 27.87 ATOM 9387 CD LYS 1389 -27.114 -7.824 61.556 1.00 27.87 ATOM 9388 CB LYS 1389 -27.757 -8.133 64.203 1.00 38.20 ATOM 9388 CC LYS 1389 -27.757 -8.133 64.203 1.00 38.20 ATOM 9389 NZ LYS 1389 -27.758 -7.817 65.056 1.00 27.87 ATOM 9390 C LYS 1389 -27.758 -7.817 65.056 1.00 26.60 ATOM 9391 C LYS 1389 -27.758 -7.817 65.056 1.00 26.60 ATOM 9391 C LYS 1389 -27.758 -7.817 65.056 1.00 26.60 ATOM 9393 CA ARG 1390 -28.980 -5.216 69.608 1.00 26.60 ATOM 9393 CA ARG 1390 -28.866 -5.541 99.910 1.00 44.99 ATOM 9393 CA ARG 1390 -28.980 -5.216 69.608 1.00 26.60 ATOM 9394 CB ARG 1390 -28.980 -5.216 69.608 1.00 26.60 ATOM 9397 NE ARG 1390 -28.980 -5.216 69.608 1.00 24.32 ATOM 9400 NHZ ARG 1390 -28.980 -5.216 69.608 1.00 24.32 ATOM 9401 C ARG 1390 -28.980 -5.216 69.608 1.00 24.32 ATOM 9402 C ARG 1390 -28.980 -5.216 69.608 1.00 24.32 ATOM 9403 N ILE 1391 -26.606 -5.541 50.00 24.33 ATOM 9404 CA LIE 1391 -26.606 -5.541 50.00 24.39 ATOM 9405 CB ILE 1391 -26.606 -5.541 50.00 24.39 ATOM 9406 CC LIE 1391 -26.606 -5.541 50.00 24.39 ATOM 9407 CGI ILE 1391 -26.609 -7.114 56.625 | | | | | | | | | |
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| ATOM 9375 CD2 LEU 1387 -24.876 -1.369 59.391 1.00 33.03 ATOM 9376 C LEU 1387 -25.019 -4.148 61.128 1.00 26.22 ATOM 9377 O LEU 1387 -25.637 -4.338 60.079 1.00 24.83 ATOM 9378 N ALA 1388 -24.082 -4.982 61.572 1.00 24.74 ATOM 9389 N ALA 1388 -22.758 -6.199 60.846 1.00 23.61 ATOM 9380 CB ALA 1388 -22.758 -6.199 60.648 1.00 23.61 ATOM 9381 C ALA 1388 -25.301 -7.517 59.60 1.00 21.94 ATOM 9382 O ALA 1388 -25.301 -7.517 59.60 1.00 20.30 ATOM 9383 N LYS 1389 -25.844 -7.096 61.705 1.00 27.87 ATOM 9384 CA LYS 1389 -27.853 -7.694 62.992 1.00 27.87 ATOM 9385 CB LYS 1389 -27.853 -7.694 62.992 1.00 32.12 ATOM 9386 CG LYS 1389 -27.057 -8.133 64.203 1.00 38.20 ATOM 9387 CD LYS 1389 -27.755 -6.500 1.00 41.46 ATOM 9388 CE LYS 1389 -27.755 -7.773 65.500 1.00 41.46 ATOM 9389 NZ LYS 1389 -27.758 -7.773 65.500 1.00 41.46 ATOM 9380 C LYS 1389 -27.758 -7.847 67.999 1.00 44.99 ATOM 9390 C LYS 1389 -27.588 -7.817 67.999 1.00 44.99 ATOM 9391 O LYS 1389 -27.588 -7.817 67.999 1.00 44.99 ATOM 9392 N ARG 1390 -28.890 -5.216 59.608 1.00 26.60 ATOM 9393 CA ARG 1390 -28.890 -5.216 59.608 1.00 26.601 ATOM 9395 CG ARG 1390 -28.890 -5.216 59.608 1.00 26.601 ATOM 9397 NE ARG 1390 -28.890 -5.216 59.608 1.00 33.06 ATOM 9398 NIL ARG 1390 -28.890 -5.216 59.608 1.00 33.66 ATOM 9399 NIL ARG 1390 -28.896 -3.255 61.570 1.00 31.81 ATOM 9390 NIL ARG 1390 -28.990 -5.216 59.608 1.00 33.66 ATOM 9391 C ARG 1390 -28.990 -5.266 59.608 1.00 33.40 ATOM 9390 NIL ARG 1390 -28.990 -5.266 59.608 1.00 33.40 ATOM 9401 C ARG 1390 -28.966 5.541 58.175 1.00 24.93 ATOM 9402 C ARG 1390 -28.966 5.541 58.175 1.00 24.93 ATOM 9404 CA ILE 1391 -26.6736 -5.663 56.570 1.00 23.57 ATOM 9405 CB ILE 1391 -26.6736 -5.663 56.570 1.00 23.53 ATOM 9406 CG2 ILE 1391 -26.6736 -5.663 56.570 1.00 23.93 ATOM 9407 CG1 ILE 1391 -26.6736 -5.663 56.570 1.00 23.93 ATOM 9408 CD1 ILE 1391 -26.6790 -7.114 56.863 1.00 30.93 ATOM 9408 CD1 ILE 1391 -26.6790 -7.114 56.803 1.00 24.93 ATOM 9408 CD1 ILE 1391 -26.6790 -7.114 56.803 1.00 24.93 ATOM 9408 CD1 ILE 1391 -26.6790 -7.114 56.803 1.00 24.95 ATOM 9408 CD1 I | | | | | | | | | |
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| ATOM 9378 N ALA 1388 -24.082 -4.982 61.572 1.00 24.74 ATOM 9379 CA ALA 1388 -22.758 -6.199 60.846 1.00 23.61 ATOM 9380 CB ALA 1388 -22.736 -7.022 61.625 1.00 21.94 ATOM 9381 C ALA 1388 -22.758 -6.199 60.648 1.00 23.61 ATOM 9381 C ALA 1388 -22.736 -7.022 61.625 1.00 21.94 ATOM 9383 C ALA 1388 -25.041 -7.002 60.648 1.00 23.83 ATOM 9383 N LYS 1389 -25.844 -7.096 61.705 1.00 25.43 ATOM 9384 CA LYS 1389 -25.844 -7.096 61.705 1.00 25.43 ATOM 9385 CB LYS 1389 -27.114 -7.824 61.656 1.00 27.87 ATOM 9386 CB LYS 1389 -27.853 -7.694 62.992 1.00 32.12 ATOM 9387 CD LYS 1389 -27.057 -8.133 64.203 1.00 38.20 ATOM 9388 CE LYS 1389 -27.057 -8.133 64.203 1.00 41.46 ATOM 9389 NZ LYS 1389 -27.773 -7.773 65.500 1.00 44.99 ATOM 9389 NZ LYS 1389 -27.588 -7.817 67.999 1.00 44.99 ATOM 9390 C LYS 1389 -27.588 -7.817 67.999 1.00 44.99 ATOM 9391 C LYS 1389 -27.588 -7.817 67.999 1.00 26.01 ATOM 9393 NARG 1390 -28.160 -5.932 60.556 1.00 26.01 ATOM 9394 CB ARG 1390 -28.160 -5.932 60.556 1.00 26.01 ATOM 9395 CG ARG 1390 -28.846 -3.704 99.830 1.00 28.15 ATOM 9397 NE ARG 1390 -28.846 -3.704 99.830 1.00 28.15 ATOM 9398 NZ ARG 1390 -28.846 -3.704 99.830 1.00 28.15 ATOM 9399 NH1 ARG 1390 -28.846 0.031 61.818 1.00 33.06 ATOM 9399 NH1 ARG 1390 -29.289 -0.068 60.782 1.00 34.15 ATOM 9401 C ARG 1390 -29.289 -0.068 60.782 1.00 33.40 ATOM 9402 O ARG 1390 -29.289 -0.068 60.782 1.00 33.40 ATOM 9403 N ILE 1391 -22.271 -5.407 57.904 1.00 24.79 ATOM 9404 CA ILE 1391 -22.271 -5.407 57.904 1.00 24.79 ATOM 9405 CB ILE 1391 -22.271 -5.407 57.904 1.00 24.32 ATOM 9406 CG2 ILE 1391 -22.271 -5.407 57.904 1.00 24.32 ATOM 9407 CCI ILE 1391 -22.271 -5.407 57.904 1.00 24.75 ATOM 9408 CDI ILE 1391 -22.271 -5.407 57.904 1.00 24.75 ATOM 9409 C ILE 1391 -22.271 -5.407 57.904 1.00 24.79 ATOM 9401 C ARG 1390 -28.666 -5.541 58.175 1.00 24.79 ATOM 9404 CA ILE 1391 -22.271 -5.407 57.904 1.00 24.79 ATOM 9405 CB ILE 1391 -22.271 -5.407 57.904 1.00 24.79 ATOM 9406 CG2 ILE 1391 -22.271 -5.407 57.904 1.00 24.79 ATOM 9407 CG1 ILE 1391 -22.271 -5.407 57.904 1.00 22.87 ATOM 9408 CD1 ILE 1 | | | | | | | | | |
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| ATOM 9379 CA ALA 1388 | | | | | | | | | |
| ATOM 9381 C ALA 1388 -22.736 -7.022 61.625 1.00 21.94 ATOM 9382 O ALA 1388 -25.041 -7.002 60.648 1.00 23.83 ATOM 9383 N LYS 1389 -25.841 -7.096 61.705 1.00 25.43 ATOM 9383 C LYS 1389 -25.844 -7.096 61.705 1.00 27.87 ATOM 9385 CB LYS 1389 -27.114 -7.824 61.656 1.00 27.87 ATOM 9386 CC LYS 1389 -27.057 -8.133 64.203 1.00 32.12 ATOM 9387 CD LYS 1389 -27.057 -8.133 64.203 1.00 38.20 ATOM 9388 CE LYS 1389 -27.773 -7.773 65.500 1.00 41.46 ATOM 9388 CE LYS 1389 -27.757 -7.773 65.500 1.00 41.46 ATOM 9389 NZ LYS 1389 -27.758 -7.817 67.999 1.00 44.99 ATOM 9390 C LYS 1389 -27.588 -7.817 67.999 1.00 44.99 ATOM 9391 O LYS 1389 -28.522 -7.984 59.716 1.00 26.60 ATOM 9392 N ARG 1390 -28.160 -5.216 59.608 1.00 26.01 ATOM 9393 CA ARG 1390 -28.846 -3.704 59.830 1.00 28.15 ATOM 9395 CG ARG 1390 -28.846 -3.704 59.830 1.00 28.15 ATOM 9396 CD ARG 1390 -28.846 -3.704 59.830 1.00 28.15 ATOM 9397 NE ARG 1390 -28.846 -3.704 59.830 1.00 23.15 ATOM 9398 CZ ARG 1390 -28.846 -3.704 59.830 1.00 23.15 ATOM 9399 NH1 ARG 1390 -28.846 -3.704 59.830 1.00 23.15 ATOM 9397 NE ARG 1390 -28.846 -3.704 59.830 1.00 23.15 ATOM 9398 CZ ARG 1390 -28.846 -3.704 59.830 1.00 23.15 ATOM 9397 NE ARG 1390 -28.846 0.031 61.818 1.00 33.06 ATOM 9398 CZ ARG 1390 -28.846 0.031 61.818 1.00 33.45 ATOM 9398 CZ ARG 1390 -28.846 0.031 61.818 1.00 35.42 ATOM 9400 NH2 ARG 1390 -29.289 -0.686 60.782 1.00 33.81 ATOM 9401 C ARG 1390 -29.361 0.924 59.901 1.00 24.93 ATOM 9402 C ARG 1390 -29.394 -5.896 57.332 1.00 24.93 ATOM 9403 N ILE 1391 -27.271 -5.407 57.904 1.00 24.93 ATOM 9404 CA ILE 1391 -26.736 -5.663 56.570 1.00 24.79 ATOM 9405 CB ILE 1391 -26.670 -8.053 57.003 1.00 23.53 ATOM 9407 CGI ILE 1391 -26.690 -7.114 56.125 1.00 24.79 ATOM 9408 CD ILE 1391 -26.690 -7.114 56.125 1.00 24.79 ATOM 9409 C ILE 1391 -26.690 -7.114 56.125 1.00 24.79 ATOM 9411 N THR 1392 -26.691 -9.463 56.654 1.00 24.75 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.75 ATOM 9418 N GLU 1393 -30.505 -9.540 56.754 1.00 24.55 ATOM 9417 O THR 1392 -26.695 -9.463 56.654 1.00 24.55 ATOM 9418 N GLU 1393 -30.5 | | | | | | | | | |
| ATOM 9381 C ALA 1388 -25.041 -7.002 60.648 1.00 23.83 ATOM 9382 O ALA 1388 -25.301 -7.517 59.560 1.00 20.30 ATOM 9383 N LYS 1389 -25.844 -7.096 61.705 1.00 25.43 ATOM 9384 CA LYS 1389 -27.114 -7.824 61.656 1.00 27.87 ATOM 9385 CB LYS 1389 -27.057 -8.133 64.203 1.00 38.20 ATOM 9386 CG LYS 1389 -27.057 -8.133 64.203 1.00 38.20 ATOM 9387 CD LYS 1389 -27.057 -8.133 64.203 1.00 38.20 ATOM 9388 CE LYS 1389 -27.773 -7.773 65.500 1.00 41.46 ATOM 9389 NZ LYS 1389 -27.588 -7.817 67.999 1.00 44.99 ATOM 9389 NZ LYS 1389 -27.588 -7.817 67.999 1.00 44.99 ATOM 9389 NZ LYS 1389 -27.588 -7.817 67.999 1.00 44.99 ATOM 9390 C LYS 1389 -28.522 -7.984 59.716 1.00 26.60 ATOM 9391 O LYS 1389 -28.522 -7.984 59.716 1.00 26.01 ATOM 9393 CA ARG 1390 -28.566 -3.503 60.556 1.00 26.01 ATOM 9393 CA ARG 1390 -28.846 -3.704 59.830 1.00 25.62 ATOM 9394 CB ARG 1390 -28.846 -3.704 59.830 1.00 25.62 ATOM 9396 CD ARG 1390 -28.846 -3.704 59.830 1.00 25.62 ATOM 9397 NE ARG 1390 -28.846 -3.704 59.830 1.00 23.158 ATOM 9398 NH ARG 1390 -28.846 0.031 61.818 1.00 33.40 ATOM 9399 NH ARG 1390 -28.466 0.031 61.818 1.00 33.40 ATOM 9399 NH ARG 1390 -29.289 -0.068 60.782 1.00 33.40 ATOM 9399 NH ARG 1390 -29.384 -5.546 59.901 1.00 24.93 ATOM 9400 NH2 ARG 1390 -29.384 -5.546 59.901 1.00 24.93 ATOM 9400 NH2 ARG 1390 -29.384 -5.546 59.901 1.00 24.93 ATOM 9401 C ARG 1390 -29.346 -5.546 59.901 1.00 24.93 ATOM 9402 C ARG 1390 -29.366 -5.541 58.175 1.00 24.93 ATOM 9402 C ARG 1390 -29.366 -5.541 58.175 1.00 24.93 ATOM 9404 CA ILE 1391 -22.717 -5.407 57.904 1.00 24.32 ATOM 9405 CB ILE 1391 -22.727 -5.607 55.130 1.00 23.53 ATOM 9405 CB ILE 1391 -22.677 -5.627 55.130 1.00 23.73 ATOM 9406 CG2 ILE 1391 -22.677 -5.627 55.130 1.00 23.92 ATOM 9406 CG2 ILE 1391 -22.677 -5.627 55.130 1.00 23.97 ATOM 9406 CG2 ILE 1391 -22.677 -5.627 55.130 1.00 24.79 ATOM 9406 CG2 ILE 1391 -22.670 -5.661 -5.463 56.654 1.00 24.79 ATOM 9415 CG ILE 1391 -22.677 -5.627 55.130 1.00 22.87 ATOM 9416 C THR 1392 -26.570 -8.053 57.001 1.00 22.87 ATOM 9417 C THR 1392 -26.691 -9.463 56.654 1.00 24.75 ATOM 9418 | | | | | | | | | |
| ATOM 9382 O ALA 1388 | MOTA | 9380 | CB | ALA | 1388 | | | | |
| ATOM 9384 CA LYS 1389 -25.844 -7.096 61.705 1.00 25.43 ATOM 9385 CB LYS 1389 -27.114 -7.824 61.656 1.00 27.87 ATOM 9386 CG LYS 1389 -27.853 -7.694 62.992 1.00 32.12 ATOM 9387 CD LYS 1389 -27.057 -8.133 64.203 1.00 38.20 ATOM 9388 CE LYS 1389 -27.773 -7.773 65.500 1.00 41.46 ATOM 9389 NZ LYS 1389 -27.773 -7.773 65.500 1.00 44.99 ATOM 9389 NZ LYS 1389 -27.588 -7.817 67.999 1.00 44.99 ATOM 9390 C LYS 1389 -27.588 -7.817 67.999 1.00 26.60 ATOM 9391 O LYS 1389 -27.588 -7.817 67.999 1.00 26.60 ATOM 9392 N ARG 1390 -28.160 -5.932 60.556 1.00 26.86 ATOM 9393 CA ARG 1390 -28.160 -5.932 60.580 1.00 26.01 ATOM 9395 CG ARG 1390 -28.846 -3.704 59.830 1.00 28.15 ATOM 9396 CD ARG 1390 -28.846 -3.704 59.830 1.00 28.15 ATOM 9397 NE ARG 1390 -28.846 -3.704 59.830 1.00 28.15 ATOM 9398 CZ ARG 1390 -30.061 -2.299 61.530 1.00 31.58 ATOM 9399 NH1 ARG 1390 -30.061 -2.299 61.530 1.00 33.40 ATOM 9399 NH1 ARG 1390 -28.466 0.031 61.818 1.00 33.40 ATOM 9399 NH1 ARG 1390 -28.466 0.031 61.818 1.00 33.41 ATOM 9401 C ARG 1390 -28.566 -5.541 58.175 1.00 24.93 ATOM 9402 O ARG 1390 -28.566 -5.541 58.175 1.00 24.93 ATOM 9404 CA ILE 1391 -27.271 -5.407 57.904 1.00 24.32 ATOM 9405 CB ILE 1391 -22.528 -5.663 56.570 1.00 23.53 ATOM 9406 CG2 ILE 1391 -22.528 -5.663 56.570 1.00 23.53 ATOM 9407 CG1 ILE 1391 -22.5248 -5.277 56.501 1.00 24.32 ATOM 9408 CD1 ILE 1391 -22.5248 -5.277 56.501 1.00 22.88 ATOM 9409 C ILE 1391 -22.6690 -7.114 56.125 1.00 23.37 ATOM 9407 CG1 ILE 1391 -22.6690 -7.114 56.125 1.00 23.37 ATOM 9408 CD1 ILE 1391 -22.6691 -9.463 56.654 1.00 24.39 ATOM 9409 C ILE 1391 -22.6690 -7.114 56.125 1.00 22.88 ATOM 9401 O THR 1392 -26.6691 -9.463 56.654 1.00 24.79 ATOM 9413 CB THR 1392 -26.6691 -9.463 56.654 1.00 24.79 ATOM 9416 C THR 1392 -26.6691 -9.463 56.654 1.00 24.79 ATOM 9417 O THR 1392 -26.165 -10.362 57.801 1.00 22.87 ATOM 9418 N GLU 1393 -22.837 -10.658 55.41 1.00 25.62 ATOM 9418 N GLU 1393 -30.505 -9.540 56.754 1.00 25.62 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 25.62 | MOTA | 9381 | С | ALA | 1388 | | | | |
| ATOM 9384 CA LYS 1389 -27.114 -7.824 61.656 1.00 27.87 ATOM 9385 CB LYS 1389 -27.853 -7.694 62.992 1.00 32.12 ATOM 9387 CD LYS 1389 -27.057 -8.133 64.203 1.00 38.20 ATOM 9387 CD LYS 1389 -27.073 -7.773 65.500 1.00 41.46 ATOM 9388 CE LYS 1389 -26.986 -8.255 66.710 1.00 43.04 ATOM 9389 NZ LYS 1389 -27.588 -7.817 67.999 1.00 44.99 ATOM 9390 C LYS 1389 -27.999 -7.252 60.556 1.00 26.60 ATOM 9391 O LYS 1389 -28.522 -7.984 59.716 1.00 26.86 ATOM 9392 N ARG 1390 -28.160 -5.932 60.580 1.00 26.01 ATOM 9393 CA ARG 1390 -28.846 -3.704 59.830 1.00 25.62 ATOM 9395 CG ARG 1390 -28.846 -3.704 59.830 1.00 25.62 ATOM 9395 CD ARG 1390 -28.910 -3.255 61.284 1.00 33.06 ATOM 9397 NE ARG 1390 -30.061 -2.299 61.530 1.00 31.58 ATOM 9398 CZ ARG 1390 -30.061 -2.299 61.530 1.00 31.58 ATOM 9399 NH1 ARG 1390 -29.289 -0.068 60.727 1.00 34.15 ATOM 9399 NH1 ARG 1390 -29.289 -0.068 60.627 1.00 33.40 ATOM 9399 NH1 ARG 1390 -29.289 -0.068 60.727 1.00 33.40 ATOM 9400 NH2 ARG 1390 -28.466 0.031 61.818 1.00 33.40 ATOM 9400 NH2 ARG 1390 -28.566 -5.541 58.175 1.00 24.32 ATOM 9401 C ARG 1390 -29.394 -5.866 57.332 1.00 24.32 ATOM 9404 CA ILE 1391 -22.271 -5.407 57.904 1.00 24.79 ATOM 9405 CB ILE 1391 -22.261 50.63 56.570 1.00 24.79 ATOM 9406 CG2 ILE 1391 -22.264 -5.277 56.501 1.00 24.79 ATOM 9407 CG1 ILE 1391 -22.2661 -3.314 56.863 1.00 23.92 ATOM 9408 CD1 ILE 1391 -22.2661 -3.314 56.863 1.00 23.92 ATOM 9408 CD1 ILE 1391 -22.661 -3.314 56.863 1.00 23.92 ATOM 9408 CD1 ILE 1391 -22.661 -3.314 56.863 1.00 23.92 ATOM 9408 CD1 ILE 1391 -22.661 -3.314 56.863 1.00 23.92 ATOM 9410 O ILE 1391 -22.661 -3.314 56.6654 1.00 24.09 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9415 CG THR 1392 -26.661 -3.314 56.865 1.00 23.92 ATOM 9416 C THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9415 CG CHR 1391 -22.26.691 -9.463 56.654 1.00 24.09 ATOM 9416 C THR 1392 -26.661 -9.463 56.654 1.00 24.09 ATOM 9416 C THR 1392 -26.661 -9.463 56.654 1.00 24.09 ATOM 9416 C THR 1392 -26.661 -9.945 56.675 1.00 24.75 ATOM | MOTA | 9382 | O | ALA | 1388 | -25.301 | -7.517 | 59.560 | 1.00 20.30 |
| ATOM 9385 CB LYS 1389 | ATOM | 9383 | N | LYS | 1389 | -25.844 | -7.096 | 61.705 | 1.00 25.43 |
| ATOM 9386 CG LYS 1389 -27.057 -8.133 64.203 1.00 38.20 ATOM 9387 CD LYS 1389 -27.773 -7.773 65.500 1.00 41.46 ATOM 9388 CE LYS 1389 -27.588 -7.817 67.999 1.00 44.99 ATOM 9389 NZ LYS 1389 -27.588 -7.817 67.999 1.00 44.99 ATOM 9390 C LYS 1389 -27.588 -7.817 67.999 1.00 44.99 ATOM 9391 O LYS 1389 -27.999 -7.252 60.556 1.00 26.60 ATOM 9391 O LYS 1389 -28.522 -7.984 59.716 1.00 26.86 ATOM 9392 N ARG 1390 -28.160 -5.932 60.580 1.00 26.01 ATOM 9393 CA ARG 1390 -28.8980 -5.216 59.608 1.00 25.62 ATOM 9395 CG ARG 1390 -28.846 -3.704 59.801 1.00 28.15 ATOM 9395 CG ARG 1390 -28.846 -3.704 59.801 1.00 33.06 ATOM 9396 CD ARG 1390 -30.061 -2.299 61.530 1.00 31.58 ATOM 9398 CZ ARG 1390 -30.047 -1.150 60.627 1.00 34.15 ATOM 9399 NH1 ARG 1390 -28.466 0.031 61.818 1.00 33.40 ATOM 9399 NH1 ARG 1390 -28.466 0.031 61.818 1.00 33.40 ATOM 9400 NH2 ARG 1390 -28.466 0.031 61.818 1.00 33.40 ATOM 9400 NH2 ARG 1390 -28.566 -5.545 59.901 1.00 33.81 ATOM 9401 C ARG 1390 -29.289 -0.068 60.782 1.00 33.40 ATOM 9401 C ARG 1390 -29.361 0.924 59.901 1.00 33.81 ATOM 9404 CA LLE 1391 -22.7271 -5.407 57.904 1.00 24.32 ATOM 9404 CA LLE 1391 -22.7271 -5.407 57.904 1.00 24.32 ATOM 9404 CA LLE 1391 -22.7271 -5.407 57.904 1.00 24.32 ATOM 9406 CG2 LLE 1391 -22.7271 -5.627 55.130 1.00 23.53 ATOM 9407 CG1 LLE 1391 -22.6736 -5.663 56.570 1.00 23.53 ATOM 9408 CD1 LLE 1391 -22.098 -3.779 56.501 1.00 23.92 ATOM 9401 C TLE 1391 -22.098 -3.779 56.501 1.00 23.92 ATOM 9401 C TLE 1391 -22.098 -3.779 56.501 1.00 23.92 ATOM 9404 CA TLE 1391 -22.6650 -5.5130 1.00 23.07 ATOM 9406 CG2 LLE 1391 -22.6650 -5.5130 1.00 23.07 ATOM 9406 CG2 LLE 1391 -22.6650 -5.5130 1.00 23.07 ATOM 9406 CG2 LLE 1391 -22.6650 -5.5130 1.00 23.07 ATOM 9406 CG2 LLE 1391 -22.6650 -5.55130 1.00 23.07 ATOM 9406 CG2 LLE 1391 -22.098 -3.779 56.501 1.00 23.92 ATOM 9412 CA THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9412 CA THR 1392 -26.690 -7.114 56.125 1.00 23.92 ATOM 9414 CG1 THR 1392 -26.690 -7.114 56.125 1.00 23.92 ATOM 9415 CG THR 1392 -26.665 -10.655 57.801 1.00 24.75 ATOM 9415 CG THR 1392 -26.6 | ATOM | 9384 | CA | LYS | 1389 | -27.114 | -7.824 | 61.656 | 1.00 27.87 |
| ATOM 9387 CD LYS 1389 -27.773 -7.773 65.500 1.00 41.46 ATOM 9388 CE LYS 1389 -26.986 -8.255 66.710 1.00 43.04 ATOM 9389 NZ LYS 1389 -27.588 -7.817 67.999 1.00 44.99 ATOM 9390 C LYS 1389 -27.588 -7.817 67.999 1.00 26.60 ATOM 9391 O LYS 1389 -22.8522 -7.984 59.716 1.00 26.86 ATOM 9392 N ARG 1390 -28.160 -5.932 60.556 1.00 26.01 ATOM 9393 CA ARG 1390 -28.980 -5.216 59.608 1.00 25.62 ATOM 9394 CB ARG 1390 -28.846 -3.704 59.830 1.00 25.62 ATOM 9395 CG ARG 1390 -28.846 -3.704 59.830 1.00 28.15 ATOM 9397 NE ARG 1390 -28.8910 -3.255 61.284 1.00 33.06 ATOM 9397 NE ARG 1390 -30.061 -2.299 61.530 1.00 31.58 ATOM 9399 NH1 ARG 1390 -29.289 -0.068 60.782 1.00 33.40 ATOM 9399 NH2 ARG 1390 -29.289 -0.068 60.782 1.00 33.40 ATOM 9399 NH2 ARG 1390 -29.289 -0.068 60.782 1.00 33.81 ATOM 9400 NH2 ARG 1390 -29.289 -0.068 60.782 1.00 33.81 ATOM 9401 C ARG 1390 -29.361 0.924 59.901 1.00 33.81 ATOM 9402 O ARG 1390 -29.361 0.924 59.901 1.00 33.81 ATOM 9402 O ARG 1390 -29.394 -5.896 57.332 1.00 21.80 ATOM 9403 N ILE 1391 -22.271 -5.407 57.904 1.00 24.32 ATOM 9405 CB ILE 1391 -22.271 -5.407 57.904 1.00 24.32 ATOM 9406 CG2 ILE 1391 -22.271 -5.663 56.570 1.00 24.38 ATOM 9406 CG2 ILE 1391 -26.736 -5.663 56.570 1.00 24.38 ATOM 9409 C ILE 1391 -26.900 -7.114 56.125 1.00 24.38 ATOM 9409 C ILE 1391 -26.900 -7.114 56.125 1.00 24.38 ATOM 9409 C ILE 1391 -26.900 -7.114 56.125 1.00 22.87 ATOM 9411 N THR 1392 -26.691 -3.314 56.863 1.00 30.37 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 22.87 ATOM 9413 CB THR 1392 -26.690 -7.114 56.125 1.00 22.87 ATOM 9414 OI ILE 1391 -22.6265 -10.362 57.003 1.00 23.07 ATOM 9415 CG THR 1392 -26.661 -3.314 56.863 1.00 30.37 ATOM 9415 CG THR 1392 -26.661 -3.314 56.863 1.00 30.37 ATOM 9416 C THR 1392 -26.661 -3.314 56.863 1.00 22.87 ATOM 9416 C THR 1392 -26.665 -10.658 55.41 1.00 24.75 ATOM 9416 C THR 1392 -26.665 -10.658 55.41 1.00 24.75 ATOM 9416 C THR 1392 -26.665 -10.658 55.41 1.00 25.51 ATOM 9416 C THR 1392 -26.2669 -9.263 57.013 1.00 25.62 ATOM 9416 C THR 1392 -26.2669 -9.263 57.013 1.00 25.62 ATOM 9416 C THR 13 | MOTA | 9385 | CB | LYS | 1389 | -27.853 | -7.694 | 62.992 | 1.00 32.12 |
| ATOM 9388 CE LYS 1389 -26.986 -8.255 66.710 1.00 43.04 ATOM 9389 NZ LYS 1389 -27.588 -7.817 67.999 1.00 44.99 ATOM 9390 C LYS 1389 -27.999 -7.252 60.556 1.00 26.60 ATOM 9391 O LYS 1389 -28.522 -7.984 59.716 1.00 26.86 ATOM 9392 N ARG 1390 -28.160 -5.932 60.580 1.00 26.01 ATOM 9393 CA ARG 1390 -28.980 -5.216 59.608 1.00 25.62 ATOM 9395 CG ARG 1390 -28.846 -3.704 59.830 1.00 28.15 ATOM 9395 CG ARG 1390 -28.846 -3.704 59.830 1.00 31.58 ATOM 9396 CD ARG 1390 -30.061 -2.299 61.530 1.00 31.58 ATOM 9397 NE ARG 1390 -30.061 -2.299 61.530 1.00 31.58 ATOM 9398 CZ ARG 1390 -30.047 -1.150 60.627 1.00 33.40 ATOM 9399 NH1 ARG 1390 -28.466 0.031 61.818 1.00 35.42 ATOM 9400 NH2 ARG 1390 -29.361 0.924 59.901 1.00 33.81 ATOM 9400 C ARG 1390 -29.361 0.924 59.901 1.00 33.81 ATOM 9401 C ARG 1390 -29.361 0.924 59.901 1.00 33.81 ATOM 9402 O ARG 1390 -29.361 0.924 59.901 1.00 24.32 ATOM 9404 CA ILE 1391 -26.736 -5.663 56.570 1.00 24.73 ATOM 9405 CB ILE 1391 -26.736 -5.663 56.570 1.00 24.32 ATOM 9406 CG2 ILE 1391 -26.736 -5.663 56.570 1.00 24.32 ATOM 9408 CD1 ILE 1391 -26.736 -5.663 56.570 1.00 24.38 ATOM 9408 CD1 ILE 1391 -26.6736 -5.663 56.570 1.00 24.38 ATOM 9408 CD1 ILE 1391 -26.670 -7.383 55.001 1.00 22.88 ATOM 9408 CD1 ILE 1391 -26.670 -7.383 55.001 1.00 22.87 ATOM 9408 CD1 ILE 1391 -26.690 -7.114 56.863 1.00 30.37 ATOM 9408 CD1 ILE 1391 -26.690 -7.114 56.851 1.00 23.92 ATOM 9410 O ILE 1391 -26.690 -7.114 56.853 1.00 23.92 ATOM 9412 CA THR 1392 -26.570 -8.053 57.003 1.00 23.92 ATOM 9412 CA THR 1392 -26.565 -10.362 57.801 1.00 25.31 ATOM 9414 OG1 THR 1392 -26.691 -9.463 56.654 1.00 24.75 ATOM 9415 CG THR 1392 -26.565 -10.362 57.801 1.00 25.31 ATOM 9416 C THR 1392 -26.565 -10.362 57.801 1.00 25.81 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.62 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.62 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.654 1.00 26.650 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.654 1.00 26.50 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.654 1.00 26.50 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.654 1.00 26.50 ATOM 9420 C | MOTA | 9386 | CG | LYS | 1389 | -27.057 | -8.133 | 64.203 | 1.00 38.20 |
| ATOM 9389 NZ LYS 1389 -27.588 -7.817 67.999 1.00 44.99 ATOM 9390 C LYS 1389 -27.999 -7.252 60.556 1.00 26.60 ATOM 9391 O LYS 1389 -28.522 -7.984 59.716 1.00 26.01 ATOM 9392 N ARG 1390 -28.160 -5.932 60.580 1.00 26.01 ATOM 9393 CA ARG 1390 -28.980 -5.216 59.608 1.00 25.62 ATOM 9394 CB ARG 1390 -28.846 -3.704 59.830 1.00 28.15 ATOM 9395 CG ARG 1390 -28.846 -3.704 59.830 1.00 23.06 ATOM 9396 CD ARG 1390 -30.061 -2.299 61.530 1.00 31.58 ATOM 9397 NE ARG 1390 -30.061 -2.299 61.530 1.00 31.58 ATOM 9398 CZ ARG 1390 -30.047 -1.150 60.627 1.00 34.15 ATOM 9399 NH1 ARG 1390 -29.289 -0.068 60.782 1.00 33.40 ATOM 9399 NH1 ARG 1390 -28.466 0.031 61.818 1.00 35.42 ATOM 9400 NH2 ARG 1390 -28.566 -5.541 58.175 1.00 24.93 ATOM 9401 C ARG 1390 -28.566 -5.541 58.175 1.00 24.93 ATOM 9402 O ARG 1390 -28.566 -5.541 58.175 1.00 24.32 ATOM 9403 N ILE 1391 -27.271 -5.407 57.904 1.00 24.32 ATOM 9405 CB ILE 1391 -25.248 -5.277 56.501 1.00 24.32 ATOM 9405 CB ILE 1391 -25.248 -5.277 56.501 1.00 24.38 ATOM 9405 CB ILE 1391 -26.6736 -5.663 56.570 1.00 23.53 ATOM 9405 CB ILE 1391 -22.6776 -5.627 55.130 1.00 22.88 ATOM 9406 CG2 ILE 1391 -22.6776 -5.627 55.130 1.00 22.88 ATOM 9407 CG1 ILE 1391 -26.6736 -5.663 56.570 1.00 23.92 ATOM 9409 C ILE 1391 -26.673 -5.627 55.130 1.00 23.92 ATOM 9408 CD ILE 1391 -26.673 -5.627 55.130 1.00 23.93 ATOM 9408 CD ILE 1391 -26.677 -5.627 55.130 1.00 23.93 ATOM 9408 CD ILE 1391 -26.679 -5.627 55.130 1.00 23.93 ATOM 9408 CD ILE 1391 -26.679 -5.627 55.130 1.00 23.92 ATOM 9410 C ILE 1391 -26.690 -7.114 56.853 1.00 30.37 ATOM 9412 CA THR 1392 -26.570 -8.053 57.003 1.00 23.92 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.75 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.75 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.31 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.51 ATOM 9418 N GLU 1393 -30.505 -9.260 56.754 1.00 24.15 ATOM 9418 N GLU 1393 -30.505 -9.253 57.013 1.00 25.50 ATOM 9418 N GLU 1393 -30.505 -9.253 57.013 1.00 25.50 ATOM 9419 CA GLU 1393 -30.505 -9.253 57.013 1.00 25.50 ATOM 9420 CB GLU | MOTA | 9387 | CD | LYS | 1389 | -27.773 | -7.773 | 65.500 | 1.00 41.46 |
| ATOM 9390 C LYS 1389 | ATOM | 9388 | CE | LYS | 1389 | -26.986 | -8.255 | 66.710 | 1.00 43.04 |
| ATOM 9390 C LYS 1389 -27.999 -7.252 60.556 1.00 26.60 ATOM 9391 O LYS 1389 -28.522 -7.984 59.716 1.00 26.86 ATOM 9392 N ARG 1390 -28.160 -5.932 60.580 1.00 26.01 ATOM 9393 CA ARG 1390 -28.980 -5.216 59.608 1.00 25.62 ATOM 9394 CB ARG 1390 -28.846 -3.704 59.830 1.00 28.15 ATOM 9395 CG ARG 1390 -28.910 -3.255 61.284 1.00 33.06 ATOM 9397 NE ARG 1390 -30.061 -2.299 61.530 1.00 31.58 ATOM 9397 NE ARG 1390 -30.047 -1.150 60.627 1.00 34.15 ATOM 9398 CZ ARG 1390 -28.466 0.031 61.818 1.00 35.42 ATOM 9399 NH1 ARG 1390 -28.466 0.031 61.818 1.00 35.42 ATOM 9400 NH2 ARG 1390 -28.466 0.031 61.818 1.00 35.42 ATOM 9400 NH2 ARG 1390 -28.566 -5.541 58.175 1.00 24.93 ATOM 9402 O ARG 1390 -28.566 -5.541 58.175 1.00 24.93 ATOM 9402 O ARG 1390 -29.394 -5.896 57.332 1.00 21.80 ATOM 9404 CA ILE 1391 -27.271 -5.667 56.653 56.570 1.00 24.32 ATOM 9405 CB ILE 1391 -26.736 -5.663 56.570 1.00 24.32 ATOM 9406 CG2 ILE 1391 -22.271 -5.627 55.130 1.00 24.38 ATOM 9408 CD ILE 1391 -22.5098 -3.779 56.789 1.00 24.38 ATOM 9408 CD ILE 1391 -22.5098 -3.779 56.789 1.00 24.38 ATOM 9408 CD ILE 1391 -22.5098 -3.779 56.789 1.00 24.38 ATOM 9408 CD ILE 1391 -22.5098 -3.779 56.789 1.00 24.38 ATOM 9408 CD ILE 1391 -22.5098 -3.779 56.789 1.00 24.38 ATOM 9408 CD ILE 1391 -22.5098 -3.779 56.789 1.00 24.38 ATOM 9408 CD ILE 1391 -22.5098 -3.779 56.789 1.00 24.38 ATOM 9408 CD ILE 1391 -22.5098 -3.779 56.789 1.00 22.88 ATOM 9408 CD ILE 1391 -22.5098 -3.779 56.789 1.00 24.38 ATOM 9408 CD ILE 1391 -22.5098 -3.779 56.789 1.00 24.38 ATOM 9412 CA THR 1392 -26.507 -8.053 57.003 1.00 22.87 ATOM 9412 CA THR 1392 -26.690 -7.114 56.125 1.00 23.07 ATOM 9412 CA THR 1392 -26.563 -11.842 57.424 1.00 24.75 ATOM 9413 CB THR 1392 -26.563 -11.842 57.424 1.00 24.75 ATOM 9416 C THR 1392 -28.8133 -9.844 56.630 1.00 25.81 ATOM 9417 O THR 1392 -28.8371 -10.658 55.411 1.00 24.15 ATOM 9418 N GLU 1393 -30.505 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.254 57.966 1.00 30.65 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30 | ATOM | 9389 | NZ | LYS | 1389 | -27.588 | -7.817 | 67.999 | 1.00 44.99 |
| ATOM 9392 N ARG 1390 -28.160 -5.932 60.580 1.00 26.01 ATOM 9393 CA ARG 1390 -28.880 -5.216 59.608 1.00 25.62 ATOM 9394 CB ARG 1390 -28.846 -3.704 59.830 1.00 28.15. ATOM 9395 CG ARG 1390 -28.846 -3.704 59.830 1.00 33.06 ATOM 9395 CD ARG 1390 -28.910 -3.255 61.284 1.00 33.06 ATOM 9397 NE ARG 1390 -30.061 -2.299 61.530 1.00 31.58 ATOM 9397 NE ARG 1390 -30.047 -1.150 60.627 1.00 34.15 ATOM 9399 NH1 ARG 1390 -29.289 -0.068 60.782 1.00 33.40 ATOM 9399 NH1 ARG 1390 -29.289 -0.068 60.782 1.00 33.40 ATOM 9400 NH2 ARG 1390 -29.361 0.924 59.901 1.00 35.42 ATOM 9400 NH2 ARG 1390 -29.361 0.924 59.901 1.00 33.81 ATOM 9401 C ARG 1390 -29.366 -5.541 58.175 1.00 24.93 ATOM 9402 O ARG 1390 -29.394 -5.896 57.332 1.00 21.80 ATOM 9403 N ILE 1391 -27.271 -5.407 57.904 1.00 24.32 ATOM 9404 CA ILE 1391 -26.736 -5.663 56.570 1.00 23.53 ATOM 9405 CB ILE 1391 -26.736 -5.663 56.570 1.00 23.53 ATOM 9406 CG2 ILE 1391 -24.677 -5.627 55.130 1.00 24.79 ATOM 9408 CD1 ILE 1391 -23.661 -3.314 56.863 1.00 30.37 ATOM 9409 C ILE 1391 -22.3661 -3.314 56.863 1.00 30.37 ATOM 9409 C ILE 1391 -22.6900 -7.114 56.125 1.00 23.92 ATOM 9410 O ILE 1391 -26.570 -8.053 57.003 1.00 23.89 ATOM 9411 N THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9413 CB THR 1392 -26.661 -10.362 57.801 1.00 25.31 ATOM 9416 C THR 1392 -26.669 -9.463 56.654 1.00 24.09 ATOM 9415 CG THR 1392 -26.669 -9.463 56.654 1.00 24.09 ATOM 9416 C THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9417 O THR 1392 -26.669 -9.463 56.654 1.00 24.09 ATOM 9418 N GLU 1393 -28.131 -10.658 55.411 1.00 25.81 ATOM 9418 N GLU 1393 -30.505 -9.540 56.754 1.00 25.62 ATOM 9419 CA GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.358 -9.159 57.966 1.00 30.65 | ATOM | 9390 | С | LYS | 1389 | -27.999 | -7.252 | 60.556 | 1.00 26.60 |
| ATOM 9392 N ARG 1390 -28.160 -5.932 60.580 1.00 26.01 ATOM 9393 CA ARG 1390 -28.980 -5.216 59.608 1.00 25.62 ATOM 9394 CB ARG 1390 -28.846 -3.704 59.830 1.00 28.15 ATOM 9395 CG ARG 1390 -28.910 -3.255 61.284 1.00 33.06 ATOM 9396 CD ARG 1390 -30.061 -2.299 61.530 1.00 31.58 ATOM 9397 NE ARG 1390 -30.061 -2.299 61.530 1.00 31.58 ATOM 9398 CZ ARG 1390 -30.047 -1.150 60.627 1.00 34.15 ATOM 9398 NH1 ARG 1390 -28.466 0.31 61.818 1.00 35.42 ATOM 9399 NH1 ARG 1390 -28.466 0.31 61.818 1.00 35.42 ATOM 9400 NH2 ARG 1390 -28.566 -5.541 58.175 1.00 24.93 ATOM 9402 O ARG 1390 -28.566 -5.541 58.175 1.00 24.93 ATOM 9402 O ARG 1390 -29.394 -5.896 57.332 1.00 21.80 ATOM 9404 CA ILE 1391 -27.271 -5.407 57.904 1.00 24.32 ATOM 9405 CB ILE 1391 -26.736 -5.663 56.570 1.00 24.33 ATOM 9405 CB ILE 1391 -25.248 -5.277 56.501 1.00 24.38 ATOM 9408 CD1 ILE 1391 -25.098 -3.779 56.789 1.00 24.38 ATOM 9409 C ILE 1391 -22.690 -7.114 56.125 1.00 24.38 ATOM 9409 C ILE 1391 -22.696 -3.314 56.863 1.00 30.37 ATOM 9410 O ILE 1391 -26.500 -7.114 56.125 1.00 23.92 ATOM 9411 N THR 1392 -26.570 -8.053 57.003 1.00 23.92 ATOM 9412 CA THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9413 CB THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9413 CB THR 1392 -26.691 -9.463 56.654 1.00 24.79 ATOM 9413 CB THR 1392 -26.691 -9.463 56.654 1.00 24.79 ATOM 9414 OG1 THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9415 CG2 THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9416 C THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9417 O THR 1392 -26.669 -9.253 57.013 1.00 25.31 ATOM 9418 N GLU 1393 -28.133 -9.844 56.309 1.00 25.62 ATOM 9418 N GLU 1393 -30.505 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9419 CA GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.358 -9.159 57.966 1.00 30.65 | ATOM | 9391 | 0 | LYS | 1389 | -28.522 | -7.984 | 59.716 | 1.00 26.86 |
| ATOM 9393 CA ARG 1390 -28.980 -5.216 59.608 1.00 25.62 ATOM 9394 CB ARG 1390 -28.846 -3.704 59.830 1.00 28.15 ATOM 9395 CG ARG 1390 -28.910 -3.255 61.284 1.00 33.06 ATOM 9396 CD ARG 1390 -30.061 -2.299 61.530 1.00 31.58 ATOM 9397 NE ARG 1390 -30.047 -1.150 60.627 1.00 34.15 ATOM 9398 CZ ARG 1390 -29.289 -0.068 60.782 1.00 33.40 ATOM 9399 NH1 ARG 1390 -28.466 0.031 61.818 1.00 35.42 ATOM 9400 NH2 ARG 1390 -29.361 0.924 59.901 1.00 33.81 ATOM 9401 C ARG 1390 -28.566 -5.541 58.175 1.00 24.93 ATOM 9402 O ARG 1390 -28.566 -5.541 58.175 1.00 24.93 ATOM 9403 N ILE 1391 -27.271 -5.407 57.904 1.00 24.32 ATOM 9404 CA ILE 1391 -26.736 -5.663 56.570 1.00 23.53 ATOM 9405 CB ILE 1391 -25.248 -5.277 56.501 1.00 24.38 ATOM 9406 CG2 ILE 1391 -25.248 -5.277 56.501 1.00 24.38 ATOM 9409 C ILE 1391 -25.098 -3.779 56.789 1.00 22.88 ATOM 9409 C ILE 1391 -23.661 -3.314 56.863 1.00 30.37 ATOM 9409 C ILE 1391 -227.323 -7.383 55.001 1.00 22.87 ATOM 9410 O ILE 1391 -27.323 -7.383 55.001 1.00 22.87 ATOM 9410 O ILE 1391 -27.323 -7.383 55.001 1.00 22.87 ATOM 9411 N THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9412 CA THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9415 CB THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9416 C THR 1392 -26.263 -11.842 57.424 1.00 25.31 ATOM 9417 O THR 1392 -26.263 -11.842 57.424 1.00 25.62 ATOM 9418 N GLU 1393 -28.313 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -26.263 -11.842 57.424 1.00 25.62 ATOM 9418 N GLU 1393 -30.505 -9.253 57.013 1.00 25.62 ATOM 9419 CA GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 | | | | | | | | | 1.00 26.01 |
| ATOM 9394 CB ARG 1390 | | | | | | | | | |
| ATOM 9395 CG ARG 1390 -28.910 -3.255 61.284 1.00 33.06 ATOM 9396 CD ARG 1390 -30.061 -2.299 61.530 1.00 31.58 ATOM 9397 NE ARG 1390 -29.289 -0.068 60.782 1.00 33.40 ATOM 9398 CZ ARG 1390 -29.289 -0.068 60.782 1.00 33.40 ATOM 9399 NH1 ARG 1390 -28.466 0.031 61.818 1.00 35.42 ATOM 9400 NH2 ARG 1390 -28.466 0.031 61.818 1.00 35.42 ATOM 9401 C ARG 1390 -28.566 -5.541 58.175 1.00 24.93 ATOM 9402 O ARG 1390 -28.566 -5.541 58.175 1.00 24.93 ATOM 9402 O ARG 1390 -29.394 -5.896 57.332 1.00 21.80 ATOM 9403 N ILE 1391 -27.271 -5.407 57.904 1.00 24.32 ATOM 9404 CA ILE 1391 -26.736 -5.663 56.570 1.00 23.53 ATOM 9405 CB ILE 1391 -26.736 -5.663 56.570 1.00 23.53 ATOM 9406 CG2 ILE 1391 -24.677 -5.627 55.130 1.00 24.79 ATOM 9408 CD1 ILE 1391 -225.098 -3.779 56.789 1.00 24.38 ATOM 9408 CD1 ILE 1391 -23.661 -3.314 56.863 1.00 30.37 ATOM 9409 C ILE 1391 -26.900 -7.114 56.125 1.00 23.92 ATOM 9410 O ILE 1391 -26.900 -7.114 56.125 1.00 23.92 ATOM 9411 N THR 1392 -26.590 -7.383 55.001 1.00 23.07 ATOM 9412 CA THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9413 CB THR 1392 -26.691 -9.463 56.654 1.00 24.79 ATOM 9413 CB THR 1392 -26.691 -9.463 56.654 1.00 24.75 ATOM 9415 CG2 THR 1392 -26.691 -9.463 56.654 1.00 24.75 ATOM 9415 CG2 THR 1392 -26.691 -9.463 56.654 1.00 24.75 ATOM 9417 O THR 1392 -226.165 -10.362 57.801 1.00 25.62 ATOM 9417 O THR 1392 -228.371 -10.658 55.411 1.00 24.75 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.62 ATOM 9417 O THR 1392 -228.371 -10.658 55.411 1.00 24.15 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.61 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.358 -9.159 57.966 1.00 35.02 | | | | | | | | | |
| ATOM 9396 CD ARG 1390 -30.061 -2.299 61.530 1.00 31.58 ATOM 9397 NE ARG 1390 -30.047 -1.150 60.627 1.00 34.15 ATOM 9398 CZ ARG 1390 -29.289 -0.068 60.782 1.00 33.40 ATOM 9399 NH1 ARG 1390 -28.466 0.031 61.818 1.00 35.42 ATOM 9400 NH2 ARG 1390 -29.361 0.924 59.901 1.00 23.81 ATOM 9401 C ARG 1390 -28.566 -5.541 58.175 1.00 24.93 ATOM 9402 O ARG 1390 -29.361 0.924 59.901 1.00 24.93 ATOM 9402 O ARG 1390 -29.394 -5.896 57.332 1.00 21.80 ATOM 9403 N ILE 1391 -27.271 -5.407 57.904 1.00 24.32 ATOM 9405 CB ILE 1391 -26.736 -5.663 56.570 1.00 23.53 ATOM 9405 CB ILE 1391 -25.248 -5.277 56.501 1.00 24.79 ATOM 9406 CG2 ILE 1391 -24.677 -5.627 55.130 1.00 22.88 ATOM 9408 CD1 ILE 1391 -25.098 -3.779 56.789 1.00 24.38 ATOM 9409 C ILE 1391 -23.661 -3.314 56.863 1.00 30.37 ATOM 9410 O ILE 1391 -26.900 -7.114 56.125 1.00 23.92 ATOM 9411 N THR 1392 -26.570 -8.053 57.003 1.00 22.87 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 23.07 ATOM 9413 CB THR 1392 -26.661 -10.043 58.052 1.00 24.79 ATOM 9414 OG1 THR 1392 -26.661 -10.043 58.052 1.00 24.75 ATOM 9416 C THR 1392 -26.661 -10.043 58.052 1.00 24.75 ATOM 9416 C THR 1392 -26.663 -11.842 57.424 1.00 25.61 ATOM 9417 O THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.61 ATOM 9419 CA GLU 1393 -29.095 -9.253 57.013 1.00 25.62 ATOM 9419 CA GLU 1393 -29.095 -9.253 57.013 1.00 25.61 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 | | | | | | | | | |
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| ATOM 9400 NH2 ARG 1390 -29.361 0.924 59.901 1.00 33.81 ATOM 9401 C ARG 1390 -28.566 -5.541 58.175 1.00 24.93 ATOM 9402 O ARG 1390 -29.394 -5.896 57.332 1.00 21.80 ATOM 9403 N ILE 1391 -27.271 -5.407 57.904 1.00 24.32 ATOM 9404 CA ILE 1391 -26.736 -5.663 56.570 1.00 23.53 ATOM 9405 CB ILE 1391 -25.248 -5.277 56.501 1.00 24.79 ATOM 9406 CG2 ILE 1391 -24.677 -5.627 55.130 1.00 22.88 ATOM 9407 CG1 ILE 1391 -25.098 -3.779 56.789 1.00 24.38 ATOM 9408 CD1 ILE 1391 -23.661 -3.314 56.863 1.00 30.37 ATOM 9409 C ILE 1391 -26.900 -7.114 56.125 1.00 23.92 ATOM 9410 O ILE 1391 -27.323 -7.383 55.001 1.00 22.87 ATOM 9411 N THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9413 CB THR 1392 -26.691 -9.463 56.654 1.00 24.75 ATOM 9414 OG1 THR 1392 -26.165 -10.362 57.801 1.00 25.31 ATOM 9415 CG2 THR 1392 -26.263 -11.842 57.424 1.00 21.60 ATOM 9416 C THR 1392 -28.371 -10.658 55.411 1.00 25.62 ATOM 9417 O THR 1392 -28.371 -10.658 55.411 1.00 25.62 ATOM 9418 N GLU 1393 -28.371 -10.658 55.411 1.00 25.62 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 | | | | | | | | | |
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| ATOM 9402 O ARG 1390 -29.394 -5.896 57.332 1.00 21.80 ATOM 9403 N ILE 1391 -27.271 -5.407 57.904 1.00 24.32 ATOM 9404 CA ILE 1391 -26.736 -5.663 56.570 1.00 23.53 ATOM 9405 CB ILE 1391 -25.248 -5.277 56.501 1.00 24.79 ATOM 9406 CG2 ILE 1391 -24.677 -5.627 55.130 1.00 22.88 ATOM 9407 CG1 ILE 1391 -25.098 -3.779 56.789 1.00 24.38 ATOM 9408 CD1 ILE 1391 -23.661 -3.314 56.863 1.00 30.37 ATOM 9409 C ILE 1391 -26.900 -7.114 56.125 1.00 23.92 ATOM 9410 O ILE 1391 -27.323 -7.383 55.001 1.00 22.87 ATOM 9411 N THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9413 CB THR 1392 -26.691 -9.463 56.654 1.00 24.75 ATOM 9414 OG1 THR 1392 -26.165 -10.362 57.801 1.00 25.31 ATOM 9415 CG2 THR 1392 -26.263 -11.842 57.424 1.00 21.60 ATOM 9416 C THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.371 -10.658 55.411 1.00 25.81 ATOM 9419 CA GLU 1393 -29.095 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 | | | | | | | | | |
| ATOM 9403 N ILE 1391 -27.271 -5.407 57.904 1.00 24.32 ATOM 9404 CA ILE 1391 -26.736 -5.663 56.570 1.00 23.53 ATOM 9405 CB ILE 1391 -25.248 -5.277 56.501 1.00 24.79 ATOM 9406 CG2 ILE 1391 -24.677 -5.627 55.130 1.00 22.88 ATOM 9407 CG1 ILE 1391 -25.098 -3.779 56.789 1.00 24.88 ATOM 9408 CD1 ILE 1391 -23.661 -3.314 56.863 1.00 30.37 ATOM 9409 C ILE 1391 -26.900 -7.114 56.125 1.00 23.92 ATOM 9410 O ILE 1391 -27.323 -7.383 55.001 1.00 22.87 ATOM 9411 N THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9413 CB THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9414 OG1 THR 1392 -26.165 -10.362 57.801 1.00 25.31 ATOM 9415 CG2 THR 1392 -26.263 -11.842 57.424 1.00 21.60 ATOM 9416 C THR 1392 -28.371 -10.658 55.411 1.00 25.62 ATOM 9417 O THR 1392 -28.371 -10.658 55.411 1.00 25.81 ATOM 9418 N GLU 1393 -29.095 -9.253 57.063 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 | | | | | | | | | |
| ATOM 9404 CA ILE 1391 -26.736 -5.663 56.570 1.00 23.53 ATOM 9405 CB ILE 1391 -25.248 -5.277 56.501 1.00 24.79 ATOM 9406 CG2 ILE 1391 -24.677 -5.627 55.130 1.00 22.88 ATOM 9407 CG1 ILE 1391 -25.098 -3.779 56.789 1.00 24.38 ATOM 9408 CD1 ILE 1391 -23.661 -3.314 56.863 1.00 30.37 ATOM 9409 C ILE 1391 -26.900 -7.114 56.125 1.00 23.92 ATOM 9410 O ILE 1391 -27.323 -7.383 55.001 1.00 22.87 ATOM 9411 N THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9414 OG1 THR 1392 -26.165 -10.362 57.801 1.00 25.31 ATOM 9415 CG2 THR 1392 -26.263 -11.842 57.424 1.00 21.60 ATOM 9416 C THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.371 -10.658 55.411 1.00 25.81 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.554 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 | | | | | | | | | |
| ATOM 9405 CB ILE 1391 -25.248 -5.277 56.501 1.00 24.79 ATOM 9406 CG2 ILE 1391 -24.677 -5.627 55.130 1.00 22.88 ATOM 9407 CG1 ILE 1391 -25.098 -3.779 56.789 1.00 24.38 ATOM 9408 CD1 ILE 1391 -23.661 -3.314 56.863 1.00 30.37 ATOM 9409 C ILE 1391 -26.900 -7.114 56.125 1.00 23.92 ATOM 9410 O ILE 1391 -27.323 -7.383 55.001 1.00 22.87 ATOM 9411 N THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9413 CB THR 1392 -26.165 -10.362 57.801 1.00 25.31 ATOM 9414 OG1 THR 1392 -26.165 -10.362 57.801 1.00 25.31 ATOM 9415 CG2 THR 1392 -26.263 -11.842 57.424 1.00 24.75 ATOM 9416 C THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.51 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | | | | | | | | | |
| ATOM 9406 CG2 ILE 1391 -24.677 -5.627 55.130 1.00 22.88 ATOM 9407 CG1 ILE 1391 -25.098 -3.779 56.789 1.00 24.38 ATOM 9408 CD1 ILE 1391 -23.661 -3.314 56.863 1.00 30.37 ATOM 9409 C ILE 1391 -26.900 -7.114 56.125 1.00 23.92 ATOM 9410 O ILE 1391 -27.323 -7.383 55.001 1.00 22.87 ATOM 9411 N THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9413 CB THR 1392 -26.165 -10.362 57.801 1.00 25.31 ATOM 9414 OG1 THR 1392 -26.165 -10.362 57.801 1.00 25.31 ATOM 9415 CG2 THR 1392 -26.263 -11.842 57.424 1.00 24.75 ATOM 9416 C THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.371 -10.658 55.411 1.00 25.62 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.51 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | | | | | | | | | |
| ATOM 9407 CG1 ILE 1391 -25.098 -3.779 56.789 1.00 24.38 ATOM 9408 CD1 ILE 1391 -23.661 -3.314 56.863 1.00 30.37 ATOM 9409 C ILE 1391 -26.900 -7.114 56.125 1.00 23.92 ATOM 9410 O ILE 1391 -27.323 -7.383 55.001 1.00 22.87 ATOM 9411 N THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9413 CB THR 1392 -26.165 -10.362 57.801 1.00 25.31 ATOM 9414 OG1 THR 1392 -26.165 -10.362 57.801 1.00 25.31 ATOM 9415 CG2 THR 1392 -26.263 -11.842 57.424 1.00 21.60 ATOM 9416 C THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.371 -10.658 55.411 1.00 25.81 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | | | | | | | | | |
| ATOM 9408 CD1 ILE 1391 -23.661 -3.314 56.863 1.00 30.37 ATOM 9409 C ILE 1391 -26.900 -7.114 56.125 1.00 23.92 ATOM 9410 O ILE 1391 -27.323 -7.383 55.001 1.00 22.87 ATOM 9411 N THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9413 CB THR 1392 -26.165 -10.362 57.801 1.00 25.31 ATOM 9414 OG1 THR 1392 -26.165 -10.362 57.801 1.00 24.75 ATOM 9415 CG2 THR 1392 -26.263 -11.842 57.424 1.00 21.60 ATOM 9416 C THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.371 -10.658 55.411 1.00 25.81 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | | | | | | | | | |
| ATOM 9409 C ILE 1391 -26.900 -7.114 56.125 1.00 23.92 ATOM 9410 O ILE 1391 -27.323 -7.383 55.001 1.00 22.87 ATOM 9411 N THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9413 CB THR 1392 -26.165 -10.362 57.801 1.00 25.31 ATOM 9414 OG1 THR 1392 -26.165 -10.362 57.801 1.00 24.75 ATOM 9415 CG2 THR 1392 -24.790 -10.043 58.052 1.00 24.75 ATOM 9416 C THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.371 -10.658 55.411 1.00 25.81 ATOM 9418 N GLU 1393 -29.95 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | | | | | | | | | |
| ATOM 9410 O ILE 1391 -27.323 -7.383 55.001 1.00 22.87 ATOM 9411 N THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9413 CB THR 1392 -26.165 -10.362 57.801 1.00 25.31 ATOM 9414 OG1 THR 1392 -24.790 -10.043 58.052 1.00 24.75 ATOM 9415 CG2 THR 1392 -26.263 -11.842 57.424 1.00 21.60 ATOM 9416 C THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.371 -10.658 55.411 1.00 24.15 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | | | | | | | | | |
| ATOM 9411 N THR 1392 -26.570 -8.053 57.003 1.00 23.07 ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9413 CB THR 1392 -26.165 -10.362 57.801 1.00 25.31 ATOM 9414 OG1 THR 1392 -24.790 -10.043 58.052 1.00 24.75 ATOM 9415 CG2 THR 1392 -26.263 -11.842 57.424 1.00 21.60 ATOM 9416 C THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.371 -10.658 55.411 1.00 24.15 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | | | | | | | | | |
| ATOM 9412 CA THR 1392 -26.691 -9.463 56.654 1.00 24.09 ATOM 9413 CB THR 1392 -26.165 -10.362 57.801 1.00 25.31 ATOM 9414 OG1 THR 1392 -24.790 -10.043 58.052 1.00 24.75 ATOM 9415 CG2 THR 1392 -26.263 -11.842 57.424 1.00 21.60 ATOM 9416 C THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.371 -10.658 55.411 1.00 24.15 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | | | | | | | | | |
| ATOM 9413 CB THR 1392 -26.165 -10.362 57.801 1.00 25.31 ATOM 9414 OG1 THR 1392 -24.790 -10.043 58.052 1.00 24.75 ATOM 9415 CG2 THR 1392 -26.263 -11.842 57.424 1.00 21.60 ATOM 9416 C THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.371 -10.658 55.411 1.00 24.15 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | | | | | | | | | |
| ATOM 9414 OG1 THR 1392 -24.790 -10.043 58.052 1.00 24.75 ATOM 9415 CG2 THR 1392 -26.263 -11.842 57.424 1.00 21.60 ATOM 9416 C THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.371 -10.658 55.411 1.00 24.15 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | | | | | | | | | |
| ATOM 9415 CG2 THR 1392 -26.263 -11.842 57.424 1.00 21.60 ATOM 9416 C THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.371 -10.658 55.411 1.00 24.15 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | | | | | | | | | |
| ATOM 9416 C THR 1392 -28.133 -9.844 56.309 1.00 25.62 ATOM 9417 O THR 1392 -28.371 -10.658 55.411 1.00 24.15 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | MOTA | 9414 | OG1 | THR | 1392 | | | | |
| ATOM 9417 O THR 1392 -28.371 -10.658 55.411 1.00 24.15 ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | MOTA | 9415 | CG2 | THR | 1392 | -26.263 | -11.842 | 57.424 | 1.00 21.60 |
| ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | ATOM | 9416 | С | THR | 1392 | | | 56.309 | |
| ATOM 9418 N GLU 1393 -29.095 -9.253 57.013 1.00 25.81 ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | MOTA | 9417 | 0 | THR | 1392 | -28.371 | -10.658 | 55.411 | 1.00 24.15 |
| ATOM 9419 CA GLU 1393 -30.505 -9.540 56.754 1.00 28.50 ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | ATOM | | N | | 1393 | | | 57.013 | 1.00 25.81 |
| ATOM 9420 CB GLU 1393 -31.358 -9.159 57.966 1.00 30.65 ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | MOTA | | CA | | | -30.505 | -9.540 | 56.754 | 1.00 28.50 |
| ATOM 9421 CG GLU 1393 -31.271 -10.140 59.124 1.00 35.02 | | | | | | | | | |
| | | | | | | | | | |
| | | | | | | | | 60.300 | 1.00 38.65 |

| MOTA | 9423 | OE1 | GLU | 1393 | -33.335 | -9.449 | 60.089 | 1.00 40.37 | |
|------|------|-----|-------------|------|---------|---------|--------|------------|---|
| | 9424 | | | | | | | 1.00 39.76 | |
| MOTA | | | GLU | 1393 | -31.602 | -9.652 | 61.435 | | |
| ATOM | 9425 | С | GLU | 1393 | -31.038 | -8.818 | 55.520 | 1.00 27.06 | |
| MOTA | 9426 | 0 | GLU | 1393 | -31.907 | -9.337 | 54.820 | 1.00 28.64 | |
| MOTA | 9427 | N | ALA | 1394 | -30.515 | -7.627 | 55.254 | 1.00 24.47 | |
| ATOM | 9428 | CA | ALA | 1394 | -30.961 | -6.847 | 54.110 | 1.00 24.04 | |
| | | | | | | | | | |
| MOTA | 9429 | CB | ALA | 1394 | -30.508 | -5.394 | 54.265 | 1.00 22.66 | |
| MOTA | 9430 | C | ALA | 1394 | -30.467 | -7.411 | 52.782 | 1.00 24.13 | |
| ATOM | 9431 | 0 | ALA | 1394 | -31.165 | -7.322 | 51.768 | 1.00 22.55 | |
| | 9432 | N | LEU | 1395 | -29.270 | -7.995 | 52.790 | 1.00 23.16 | |
| ATOM | | | | | | | | | |
| ATOM | 9433 | CA | LEU | 1395 | -28.682 | -8.551 | 51.571 | 1.00 22.35 | |
| ATOM | 9434 | CB | LEU | 1395 | -27.169 | -8.307 | 51.557 | 1.00 23.06 | |
| ATOM | 9435 | CG | LEU | 1395 | -26.678 | -6.859 | 51.608 | 1.00 24.33 | |
| ATOM | 9436 | | LEU | 1395 | -25.165 | -6.854 | 51.357 | 1.00 23.88 | |
| | | | | | | | | 1.00 26.78 | |
| MOTA | 9437 | | LEU | 1395 | -27.386 | -6.016 | 50.579 | | |
| MOTA | 9438 | С | LEU | 1395 | -28.939 | -10.036 | 51.352 | 1.00 20.89 | |
| ATOM | 9439 | 0 | LEU | 1395 | -28.995 | -10.815 | 52.298 | 1.00 20.06 | |
| ATOM | 9440 | N | ALA | 1396 | -29.091 | -10.416 | 50.085 | 1.00 20.42 | |
| | 9441 | CA | ALA | 1396 | | -11.805 | 49.716 | 1.00 21.29 | |
| MOTA | | | | | | | | | |
| MOTA | 9442 | CB | ALA | 1396 | | -11.871 | 48.413 | 1.00 19.07 | |
| ATOM | 9443 | С | ALA | 1396 | -28.005 | -12.548 | 49.552 | 1.00 20.66 | |
| MOTA | 9444 | 0 | ALA | 1396 | -27.916 | -13.753 | 49.809 | 1.00 19.21 | |
| ATOM | 9445 | N | ILE | 1397 | | -11.823 | 49.116 | 1.00 19.78 | |
| | | | | | | | | | |
| MOTA | 9446 | CA | ILE | 1397 | | -12.405 | 48.933 | 1.00 20.20 | |
| MOTA | 9447 | CB | ILE | 1397 | -24.721 | -11.463 | 48.134 | 1.00 19.10 | |
| MOTA | 9448 | CG2 | ILE | 1397 | -25.280 | -11.237 | 46.742 | 1.00 19.43 | |
| ATOM | 9449 | | ILE | 1397 | | -10.139 | 48.875 | 1.00 17.71 | |
| | | | | | | | | 1.00 18.82 | |
| MOTA | 9450 | | ILE | 1397 | -23.568 | -9.181 | 48.227 | | |
| ATOM | 9451 | С | ILE | 1397 | -25.020 | -12.649 | 50.299 | 1.00 20.56 | |
| ATOM | 9452 | 0 | ILE | 1397 | -25.389 | -12.008 | 51.282 | 1.00 21.78 | |
| ATOM | 9453 | N | PRO | 1398 | -24.066 | -13.586 | 50.381 | 1.00 22.06 | |
| | 9454 | CD | | | | -14.529 | 49.342 | 1.00 22.24 | |
| ATOM | | | PRO | 1398 | | | | | |
| MOTA | 9455 | CA | PRO | 1398 | | -13.871 | 51.661 | 1.00 22.34 | - |
| ATOM | 9456 | CB | PRO | 1398 | -22.633 | -15.150 | 51.373 | 1.00 23.09 | |
| MOTA | 9457 | CG | PRO | 1398 | -22.353 | -15.057 | 49.917 | 1.00 26.50 | |
| ATOM | 9458 | C | PRO | 1398 | | -12.728 | 52.168 | 1.00 21.87 | |
| | | | | | | | | | |
| MOTA | 9459 | 0 | PRO | 1398 | | -12.075 | 51.394 | 1.00 21.73 | |
| MOTA | 9460 | N | VAL | 1399 | -22.621 | -12.479 | 53.472 | 1.00 21.04 | |
| MOTA | 9461 | CA | VAL | 1399 | -21.845 | -11.423 | 54.102 | 1.00 20.62 | |
| ATOM | 9462 | CB | VAL | 1399 | | -10.465 | 54.918 | 1.00 21.23 | |
| | | | | | | | 55.569 | 1.00 20.53 | |
| MOTA | 9463 | | VAL | 1399 | -21.906 | -9.373 | | | |
| MOTA | 9464 | CG2 | VAL | 1399 | -23.796 | -9.833 | 54.007 | 1.00 21.96 | |
| MOTA | 9465 | С | VAL | 1399 | -20.793 | -12.033 | 55.021 | 1.00 20.44 | |
| MOTA | 9466 | 0 | VAL | 1399 | -21.115 | -12.798 | 55.938 | 1.00 19.55 | |
| ATOM | 9467 | N | ILE | 1400 | | -11.694 | 54.751 | 1.00 20.90 | |
| | | | | | | | | | |
| MOTA | 9468 | CA | ILE | 1400 | | -12.181 | 55.522 | 1.00 19.21 | |
| MOTA | 9469 | CB | $_{ m ILE}$ | 1400 | -17.218 | -12.559 | 54.590 | 1.00 20.36 | |
| ATOM | 9470 | CG2 | ILE | 1400 | -16.008 | -12.966 | 55.418 | 1.00 20.56 | |
| MOTA | 9471 | CG1 | ILE | 1400 | -17.643 | -13.705 | 53.668 | 1.00 22.22 | |
| ATOM | 9472 | CD1 | ILE | 1400 | | -14.082 | 52.643 | 1.00 24.06 | |
| | | | | | | | | | _ |
| ATOM | 9473 | С | ILE | 1400 | | -11.083 | 56.462 | 1.00 19.24 | |
| MOTA | 9474 | 0 | ILE | 1400 | -17.585 | -9.985 | 56.026 | 1.00 17.97 | |
| ATOM | 9475 | N | GLY | 1401 | -17.898 | -11.380 | 57.754 | 1.00 17.48 | |
| ATOM | 9476 | CA | GLY | 1401 | | -10.368 | 58.700 | 1.00 17.76 | |
| ATOM | 9477 | C | GLY | 1401 | | -10.615 | 59.429 | 1.00 17.82 | |
| | | | | | | | | | |
| ATOM | 9478 | 0 | GLY | 1401 | -15.731 | | 59.583 | 1.00 18.37 | |
| MOTA | 9479 | N | ILE | 1402 | -15.567 | -9.519 | 59.846 | 1.00 17.14 | |
| MOTA | 9480 | CA | ILE | 1402 | -14.342 | -9.549 | 60.622 | 1.00 19.20 | |
| ATOM | 9481 | CB | ILE | 1402 | -13.061 | -9.437 | 59.731 | 1.00 17.10 | |
| | 9482 | CG2 | | 1402 | -13.207 | -8.319 | 58.708 | 1.00 19.67 | |
| ATOM | | | ILE | | | | | | |
| ATOM | 9483 | CG1 | ILE | 1402 | -11.844 | -9.222 | 60.626 | 1.00 22.25 | |
| ATOM | 9484 | CD1 | ILE | 1402 | -10.521 | -9.488 | 59.939 | 1.00 21.22 | |
| ATOM | 9485 | С | ILE | 1402 | -14.477 | -8.359 | 61.562 | 1.00 17.66 | |
| ATOM | 9486 | ō | ILE | 1402 | -14.489 | -7.202 | 61.134 | 1.00 21.00 | |
| | | | | | -14.616 | -8.646 | 62.849 | 1.00 18.73 | |
| ATOM | 9487 | N | GLY | 1403 | | | | | |
| ATOM | 9488 | CA | GLY | 1403 | -14.800 | -7.572 | 63.805 | 1.00 19.62 | |
| MOTA | 9489 | С | GLY | 1403 | -16.208 | -7.017 | 63.675 | 1.00 20.89 | |
| ATOM | 9490 | 0 | GLY | 1403 | -16.457 | -5.837 | 63.934 | 1.00 20.69 | |
| ATOM | 9491 | N | ALA | 1404 | -17.137 | -7.871 | 63.259 | 1.00 20.95 | |
| | | | | | | | | | |
| MOTA | 9492 | CA | ALA | 1404 | -18.529 | -7.452 | 63.100 | 1.00 22.83 | |
| MOTA | 9493 | CB | ALA | 1404 | -18.881 | -7.354 | 61.614 | 1.00 24.62 | |
| MOTA | 9494 | С | ALA | 1404 | -19.502 | -8.391 | 63.807 | 1.00 24.35 | |
| ATOM | 9495 | ō | ALA | 1404 | -20.706 | -8.344 | 63.558 | 1.00 24.70 | |
| | | | | | | -9.246 | 64.685 | 1.00 24.62 | |
| ATOM | 9496 | N | GLY | 1405 | -18.980 | | | | |
| ATOM | 9497 | CA | GLY | 1405 | -19.833 | | 65.411 | 1.00 25.54 | |
| ATOM | 9498 | C | GLY | 1405 | -20.075 | | 64.683 | | |
| MOTA | 9499 | 0 | GLY | 1405 | -19.573 | -11.681 | 63.581 | 1.00 27.10 | |
| | | | | | | | | | |
| | | | | | | | | | |

| ATOM | 9500 | N | ASN | 1406 | -20.854 | -12.367 | 65.297 | 1.00 25.69 |
|--------------|--------------|------------|------------|--------------|--------------------|--------------------|------------------|--------------------------|
| MOTA | 9501 | CA | ASN | 1406 | -21.149 | | 64.701 | 1.00 25.78 |
| MOTA | 9502 | CB | ASN | 1406 | -21.144 | | 65.781 | 1.00 26.59 |
| ATOM | 9503 | CG | ASN | 1406 | -22.323 | | 66.745 | 1.00 28.85 |
| MOTA | 9504 | OD1 | | 1406 | -22.638 -22.972 | | 67.470 | 1.00 29.88 1.00 25.54 |
| ATOM ATOM | 9505 9506 | ND2 C | ASN ASN | 1406 1406 | -22.972 -22.481 | | 66.760 63.952 | 1.00 25.54 1.00 24.77 |
| ATOM | 9507 | 0 | ASN | 1406 | -22.461 | | 63.579 | 1.00 25.44 |
| ATOM | 9508 | N | VAL | 1407 | -23.071 | | 63.725 | 1.00 24.74 |
| ATOM | 9509 | CA | VAL | 1407 | -24.354 | | 63.033 | 1.00 25.37 |
| ATOM | 9510 | CB | VAL | 1407 | -25.064 | | 63.402 | 1.00 25.71 |
| MOTA | 9511 | CG1 | VAL | 1407 | -26.505 | -11.144 | 62.893 | 1.00 31.10 |
| MOTA | 9512 | CG2 | VAL | 1407 | -25.040 | | 64.913 | 1.00 27.35 |
| MOTA | 9513 | C | VAL | 1407 | -24.224 | | 61.512 | 1.00 25.31 |
| MOTA | 9514 | 0 | VAL | 1407 | -25.223 | | 60.790 | 1.00 24.78 |
| MOTA | 9515 | N | THR | 1408 | -22.991 -22.753 | | 61.024 59.591 | 1.00 23.39 1.00 21.03 |
| ATOM ATOM | 9516 9517 | CA CB | THR THR | 1408 1408 | -21.375 | | 59.238 | 1.00 21.03 |
| ATOM | 9518 | | THR | 1408 | -20.354 | | 60.064 | 1.00 19.12 |
| ATOM | 9519 | | THR | 1408 | -21.401 | | 59.460 | 1.00 17.17 |
| ATOM | 9520 | C | THR | 1408 | -22.813 | | 59.104 | 1.00 21.73 |
| ATOM | 9521 | 0 | THR | 1408 | -22.821 | -14.867 | 59.908 | 1.00 24.16 |
| MOTA | 9522 | N | ASP | 1409 | -22.874 | -14.090 | 57.785 | 1.00 19.78 |
| MOTA | 9523 | CA | ASP | 1409 | -22.942 | | 57.157 | 1.00 19.91 |
| MOTA | 9524 | CB | ASP | 1409 | -23.371 | | 55.696 | 1.00 21.36 |
| ATOM | 9525 | CG CD1 | ASP | 1409 | -24.712 | | 55.553 | 1.00 22.44 |
| MOTA | 9526 | OD1 OD2 | | 1409 1409 | -25.693 -24.786 | | 56.107 54.899 | 1.00 22.97 1.00 25.06 |
| ATOM ATOM | 9527 9528 | C | ASP ASP | 1409 | -24.780 | | 57.211 | 1.00 23.00 |
| ATOM | 9529 | 0 | ASP | 1409 | -21.533 | | 57.236 | 1.00 18.44 |
| MOTA | 9530 | N | GLY | 1410 | -20.534 | | 57.219 | 1.00 21.88 |
| ATOM | 9531 | CA | GLY | 1410 | -19.204 | | 57.269 | 1.00 20.44 |
| MOTA | 9532 | С | GLY | 1410 | -18.249 | -15.097 | 58.124 | 1.00 19.85 |
| ATOM | 9533 | 0 | GLY | 1410 | -18.589 | | 58.594 | 1.00 18.97 |
| MOTA | 9534 | N | GLN | 1411 | -17.050 | | 58.322 | 1.00 19.88 |
| ATOM | 9535 | CA | GLN | 1411 | -16.011 | | 59.116 | 1.00 20.00 |
| ATOM | 9536 9537 | CB CG | GLN GLN | 1411 1411 | -15.817 -16.981 | | 60.447 61.417 | 1.00 19.91 1.00 19.40 |
| ATOM ATOM | 9538 | CD | GLN | 1411 | -17.301 | | 61.801 | 1.00 15.40 |
| ATOM | 9539 | OE1 | | 1411 | -16.414 | | 62.153 | 1.00 18.73 |
| ATOM | 9540 | NE2 | | 1411 | -18.578 | | 61.752 | 1.00 18.43 |
| ATOM | 9541 | С | GLN | 1411 | -14.676 | | 58.382 | 1.00 20.57 |
| MOTA | 9542 | 0 | GLN | 1411 | -14.421 | -15.889 | 57.558 | 1.00 19.66 |
| MOTA | 9543 | N | ILE | 1412 | -13.824 | | 58.697 | 1.00 22.26 |
| MOTA | 9544 | CA | ITÉ | 1412 | -12.501 | | 58.097 | 1.00 23.53 |
| ATOM | 9545 | CB | ILE | 1412 | -12.530 | 4 | 56.776 | 1.00 23.95 |
| MOTA | 9546 9547 | CG2 CG1 | ILE ILE | 1412 1412 | -12.737 -11.227 | -11.675 | 57.075 56.010 | 1.00 24.56 1.00 25.80 |
| ATOM ATOM | 9548 | CD1 | ILE | 1412 | -11.316 | | 54.543 | 1.00 25.24 |
| ATOM | 9549 | C | ILE | 1412 | -11.536 | | 59.097 | 1.00 25.52 |
| ATOM | 9550 | Ō | ILE | 1412 | | -12.627 | 60.014 | 1.00 23.69 |
| ATOM | 9551 | N | LEU | 1413 | -10.248 | -13.607 | 58.933 | 1.00 27.48 |
| MOTA | 9552 | CA | LEU | 1413 | | -13.032 | 59.815 | 1.00 28.85 |
| MOTA | 9553 | CB | LEU | 1413 | | -13.635 | 61.216 | 1.00 34.02 |
| MOTA | 9554 | CG | LEU | 1413 | | -12.665 | 62.403 | 1.00 37.41 |
| MOTA | 9555 | CD1 CD2 | | 1413 | | -13.472 -11.718 | 63.680 62.283 | 1.00 39.43 1.00 39.02 |
| MOTA MOTA | 9556 9557 | CDZ | LEU | 1413 1413 | | -13.315 | 59.243 | 1.00 33.02 |
| ATOM | 9558 | 0 | LEU | 1413 | | -14.259 | 58.470 | 1.00 25.03 |
| ATOM | 9559 | N | VAL | 1414 | | -12.485 | 59.610 | 1.00 29.11 |
| ATOM | 9560 | CA | VAL | 1414 | -5.520 | -12.662 | 59.147 | 1.00 29.08 |
| MOTA | 9561 | CB | VAL | 1414 | | -11.435 | 59.483 | 1.00 30.55 |
| MOTA | 9562 | CG1 | | 1414 | | -11.628 | 58.900 | 1.00 31.68 |
| MOTA | 9563 | CG2 | | 1414 | | -10.165 | 58.928 | 1.00 31.09 |
| ATOM | 9564 | C | VAL | 1414 | | -13.880 | 59.863 61.092 | 1.00 28.58 |
| MOTA MOTA | 9565 9566 | O N | VAL MET | 1414 1415 | | -13.928 -14.865 | 59.087 | 1.00 28.63 1.00 26.58 |
| ATOM | 9567 | CA | MET | 1415 | | -16.096 | 59.644 | 1.00 25.18 |
| ATOM | 9568 | CB | MET | 1415 | | -16.959 | 58.527 | 1.00 21.68 |
| ATOM | 9569 | CG | MET | 1415 | | -16.306 | 57.777 | 1.00 20.54 |
| MOTA | 9570 | SD | MET | 1415 | -1.043 | -17.545 | 57.300 | 1.00 21.74 |
| MOTA | 9571- | CE | MET . | 1415 | | -17.623 | 58.832 | 1.00 21.73 |
| ATOM | 9572 | C | MET | 1415 | | -15.850 | 60.713 | 1.00 25.50 |
| ATOM | 9573 | 0 | MET | 1415 | | -16.614 | 61.671 | 1.00 25.46 |
| MOTA MOTA | 9574 9575 | N CA | HIS HIS | 1416 1416 | | -14.778 -14.440 | 60.548 61.496 | 1.00 25.98 1.00 27.03 |
| ATOM | 9575 9576 | CB | HIS | 1416 | | -13.242 | 60.974 | 1.00 27.03 |
| | | | | - | | | | |

| MOTA | 9577 | CG | HIS | 1416 | 0.482 | -13.542 | 59.726 | 1.00 26.99 |
|--------------|--------------|-----------|------------|--------------|------------------|------------------|------------------|--------------------------|
| ATOM | 9578 | CD2 | HIS | 1416 | 0.121 | -13.513 | 58.421 | 1.00 25.19 |
| MOTA | 9579 | ND1 | HIS | 1416 | 1.782 | -14.002 | 59.750 | 1.00 25.73 |
| ATOM | 9580 | | HIS | 1416 | 2.188 | -14.243 | 58.517 | 1.00 24.78 |
| MOTA | 9581 | | HIS | 1416 | 1.198 | | 57.690 | 1.00 27.44 |
| ATOM | 9582 | С | HIS | 1416 | -1.651 | | 62.889 | 1.00 28.75 |
| MOTA | 9583 | 0 | HIS | 1416 | -1.076 | | 63.887 | 1.00 27.94 |
| MOTA | 9584 | N | ASP | 1417 | -2.773 | | 62.966 | 1.00 29.75 |
| ATOM | 9585 | CA | ASP | 1417 | -3.386 | | 64.262 | 1.00 33.00 |
| ATOM ATOM | 9586 9587 | CB CG | ASP | 1417 1417 | -4.458 -3.886 | | 64.134 63.731 | 1.00 34.18 1.00 37.67 |
| ATOM | 9588 | | ASP ASP | 1417 | -2.900 | | 64.361 | 1.00 37.87 |
| ATOM | 9589 | OD2 | | 1417 | -4.429 | | 62.788 | 1.00 40.11 |
| ATOM | 9590 | C | ASP | 1417 | -4.025 | | 64.848 | 1.00 33.09 |
| ATOM | 9591 | ō | ASP | 1417 | -4.130 | | 66.067 | 1.00 34.61 |
| ATOM | 9592 | N | ALA | 1418 | -4.455 | -15.312 | 63.974 | 1.00 34.01 |
| MOTA | 9593 | CA | ALA | 1418 | -5.094 | -16.552 | 64.399 | 1.00 35.06 |
| MOTA | 9594 | CB | ALA | 1418 | -5.800 | -17.207 | 63.208 | 1.00 34.52 |
| MOTA | 9595 | С | ALA | 1418 | | -17.535 | 65.034 | 1.00 36.11 |
| MOTA | 9596 | 0 | ALA | 1418 | | 18.505 | 65.671 | 1.00 36.84 |
| ATOM | 9597 | N | PHE | 1419 | | -17.287 | 64.863 | 1.00 36.18 |
| MOTA | 9598 | CA | PHE | 1419 | | -18.161 | 65.436 | 1.00 36.22 |
| MOTA | 9599 | CB | PHE | 1419 | | -18.849 | 64.322 | 1.00 37.87 |
| ATOM ATOM | 9600 9601 | CG CD1 | PHE PHE | 1419 1419 | -1.861 -2.859 | | 63.349 63.806 | 1.00 39.07 1.00 38.80 |
| ATOM | 9602 | | PHE | 1419 | -1.671 | | 61.978 | 1.00 38.80 |
| ATOM | 9603 | | PHE | 1419 | -3.654 | | 62.914 | 1.00 39.60 |
| ATOM | 9604 | | PHE | 1419 | | -20.180 | 61.075 | 1.00 39.92 |
| ATOM | 9605 | CZ | PHE | 1419 | | -21.035 | 61.546 | 1.00 40.35 |
| ATOM | 9606 | C | PHE | 1419 | | -17.412 | 66.369 | 1.00 35.97 |
| MOTA | 9607 | 0 | PHE | 1419 | 0.267 | -17.880 | 66.660 | 1.00 35.74 |
| ATOM | 9608 | N | GLY | 1.420 | -1.278 | | 66.832 | 1.00 35.56 |
| MOTA | 9609 | CA | GLY | 1420 | -0.472 | | 67.739 | 1.00 34.95 |
| MOTA | 9610 | С | GLY | 1420 | 0.900 | | 67.205 | 1.00 34.01 |
| ATOM | 9611 | 0 | GLY | 1420 | 1.762 | | 67.960 | 1.00 33.90 |
| ATOM | 9612 | N | ILE | 1421 | 1.112 | | 65.908 | 1.00 31.41 |
| MOTA | 9613 | CA | ILE | 1421 | 2.394 2.423 | | 65.299 | 1.00 28.98 |
| MOTA MOTA | 9614 9615 | CB CG2 | ILE ILE | 1421 | 3.732 | | 63.804 63.156 | 1.00 28.18 1.00 24.57 |
| ATOM | 9616 | CG1 | ILE | 1421 | 2.264 | | 63.689 | 1.00 24.57 |
| ATOM | 9617 | | ILE | 1421 | 2.034 | | 62.278 | 1.00 26.39 |
| ATOM | 9618 | C | ILE | 1421 | 2.626 | | 65.411 | 1.00 29.18 |
| ATOM | 9619 | 0 | ILE | 1421 | 3.716 | | 65.761 | 1.00 27.59 |
| ATOM | 9620 | N | THR | 1422 | 1.577 | -12.676 | 65.143 | 1.00 30.56 |
| ATOM | 9621 | CA | THR | 1422 | 1.654 | -11.222 | 65.195 | 1.00 33.09 |
| ATOM | 9622 | CB | THR | 1422 | | -10.585 | 64.796 | 1.00 34.07 |
| ATOM | ·9623 | | THR | 1422 | -0.711 | | 65.685 | 1.00 35.73 |
| ATOM | 9624 | - | THR | 1422 | -0.045 | | 63.372 | 1.00 31.21 |
| MOTA | 9625 | C | THR | 1422 | 2.055 | -10.658 | 66.552 | 1.00 35.46 |
| ATOM | 9626 | 0 | THR | 1422 | 1.761 | | 67.594 | 1.00 33.19 |
| ATOM | 9627 | N | GLY | 1423 | 2.716 3.187 | -9.503 | 66.502 | 1.00 38.12 |
| ATOM ATOM | 9628 9629 | CA C | GLY GLY | 1423 1423 | 2.958 | -8.802 -9.491 | 67.682 69.005 | 1.00 42.38 1.00 44.65 |
| ATOM | 9630 | 0 | GLY | 1423 | 3.540 | | 69.273 | 1.00 47.25 |
| ATOM | 9631 | N | GLY | 1424 | 2.113 | -8.894 | 69.838 | 1.00 45.54 |
| ATOM | 9632 | CA | GLY | 1424 | 1.826 | -9.478 | 71.133 | 1.00 46.73 |
| MOTA | 9633 | С | GLY | 1424 | 0.367 | -9.366 | 71.525 | 1.00 47.44 |
| MOTA | 9634 | 0 | GLY | 1424 | -0.242 | -10.347 | 71.953 | 1.00 48.03 |
| MOTA | 9635 | N | HIS | 1425 | -0.202 | -8.174 | 71.378 | 1.00 47.09 |
| MOTA | 9636 | CA | HIS | 1425 | -1.597 | -7.968 | 71.745 | 1.00 48.66 |
| MOTA | 9637 | CB | HIS | 1425 | -1.732 | -6.705 | 72.598 | 1.00 50.45 |
| ATOM | 9638 | CG | HIS | 1425 | -2.977 | -6.666 | 73.427 | 1.00 52.26 |
| ATOM | 9639 | | HIS | 1425 | -3.834 | -5.654 | 73.701 | 1.00 53.70 |
| ATOM | 9640 | | HIS | 1425 | -3.434 -4.518 | -7.756 | 74.136 74.812 | 1.00 53.03 1.00 52.99 |
| ATOM ATOM | 9641 9642 | | HIS HIS | 1425 1425 | -4.781 | -7.418 -6.148 | 74.566 | 1.00 54.24 |
| ATOM | 9643 | NE2 | HIS | 1425 | -2.485 | -0.146 -7.868 | 70.511 | 1.00 34.24 |
| ATOM | 9644 | 0 | HIS | 1425 | -2.627 | -6.802 | 69.917 | 1.00 46.90 |
| ATOM | 9645 | N | ILE | 1426 | -3.078 | -8.993 | 70.129 | 1.00 47.14 |
| ATOM | 9646 | CA | ILE | 1426 | -3.942 | -9.039 | 68.960 | 1.00 46.99 |
| MOTA | 9647 | CB | ILE | 1426 | -4.374 | -10.485 | 68.648 | 1.00 47.44 |
| MOTA | 9648 | CG2 | | 1426 | -3.160 | -11.313 | 68.259 | 1.00 49.26 |
| MOTA | 9649 | | ILE | 1426 | -5.069 | -11.098 | 69.860 | 1.00 47.01 |
| MOTA | 9650 | | ILE | 1426 | -5.604 | -12.486 | 69.606 | 1.00 47.10 |
| ATOM | 9651 | С | ILE | 1426 | -5.184 | -8.177 | 69.148 | 1.00 45.31 |
| ATOM | 9652 | 0 | ILE | 1426 | -5.532 | -7.801 | 70.271 | 1.00 45.25 |
| MOTA | 9653 | N | PRO | 1427 | -5.868 | -7.844 | 68.043 | 1.00 44.13 |

| ATOM | 9654 | CD | PRO | 1427 | -5.581 | -8.236 | 66.652 | 1.00 43.74 |
|------|--------------|-----|------------|------|---------|---------|--------|------------|
| ATOM | 9655 | CA | PRO | 1427 | -7.078 | -7.020 | 68.112 | 1.00 42.56 |
| ATOM | 9656 | CB | PRO | 1427 | -7.414 | -6.784 | 66.642 | 1.00 42.85 |
| ATOM | 9657 | CG | PRO | 1427 | -6.925 | -8.038 | 65.989 | 1.00 44.37 |
| ATOM | 9658 | С | PRO | 1427 | -8.212 | -7.703 | 68.870 | 1.00 40.69 |
| ATOM | 9659 | 0 | PRO | 1427 | -8.274 | -8.928 | 68.941 | 1.00 39.71 |
| ATOM | 9660 | N | LYS | 1428 | -9.105 | -6.899 | 69.436 | 1.00 39.55 |
| ATOM | 9661 | CA | LYS | 1428 | -10.238 | -7.422 | 70.189 | 1.00 38.02 |
| ATOM | 9662 | CB | LYS | 1428 | -11.155 | -6.274 | 70.631 | 1.00 40.74 |
| ATOM | 9663 | CG | LYS | 1428 | -10.693 | -5.483 | 71.860 | 1.00 44.43 |
| ATOM | 9664 | CD | LYS | 1428 | -9.402 | -4.698 | 71.629 | 1.00 46.69 |
| ATOM | 9665 | CE | LYS | 1428 | -8.168 | -5.494 | 72.046 | 1.00 47.27 |
| ATOM | 9666 | NZ | LYS | 1428 | -6.917 | -4.715 | 71.829 | 1.00 48.13 |
| ATOM | 9667 | C | LYS | 1428 | -11.065 | -8.451 | 69.418 | 1.00 35.07 |
| ATOM | 9668 | ō | LYS | 1428 | -11.557 | -9.417 | 69.999 | 1.00 33.86 |
| АТОМ | 9669 | N | PHE | 1429 | -11.213 | -8.250 | 68.112 | 1.00 32.23 |
| ATOM | 9670 | CA | PHE | 1429 | -12.014 | -9.159 | 67.293 | 1.00 28.78 |
| ATOM | 9671 | СВ | PHE | 1429 | -12.484 | -8.430 | 66.027 | 1.00 27.62 |
| ATOM | 9672 | CG | PHE | 1429 | -11.366 | -7.984 | 65.131 | 1.00 24.25 |
| ATOM | 9673 | CD1 | | 1429 | -10.713 | -8.895 | 64.304 | 1.00 23.47 |
| ATOM | 9674 | CD2 | | 1429 | -10.962 | -6.654 | 65.116 | 1.00 22.84 |
| ATOM | 9675 | CE1 | | 1429 | -9.673 | -8.489 | 63.476 | 1.00 21.56 |
| ATOM | 9676 | CE2 | | 1429 | -9.922 | -6.237 | 64.293 | 1.00 23.95 |
| ATOM | 9677 | CZ | PHE | 1429 | -9.276 | -7.156 | 63.469 | 1.00 24.89 |
| ATOM | 9678 | C | PHE | 1429 | -11.314 | | 66.914 | 1.00 28.44 |
| ATOM | 9679 | ō | PHE | 1429 | -11.952 | | 66.424 | 1.00 26.30 |
| ATOM | 9680 | N | ALA | 1430 | -10.008 | | 67.149 | 1.00 28.50 |
| ATOM | 9681 | CA | ALA | 1430 | | -11.726 | 66.816 | 1.00 29.62 |
| | 9682 | CB | ALA | 1430 | | -11.720 | 66.325 | 1.00 29.02 |
| ATOM | 9683 | С | ALA | 1430 | | -12.685 | 67.998 | 1.00 25.24 |
| ATOM | | | | | | -12.311 | 69.150 | 1.00 31.63 |
| ATOM | 9684 9685 | 0 | ALA LYS | 1430 | | -12.311 | 67.695 | 1.00 31.83 |
| ATOM | | N | | 1431 | | -13.927 | | |
| ATOM | 9686 | CA | LYS | 1431 | | | 68.712 | 1.00 32.80 |
| ATOM | 9687 | CB | LYS | 1431 | | -15.759 | 68.891 | 1.00 33.38 |
| ATOM | 9688 | CG | LYS | 1431 | | -16.878 | 69.916 | 1.00 35.77 |
| ATOM | 9689 | CD | LYS | 1431 | -11.042 | | 70.055 | 1.00 36.57 |
| ATOM | 9690 | CE | LYS | 1431 | -10.902 | | 70.998 | 1.00 37.40 |
| MOTA | 9691 | NZ | LYS | 1431 | -12.189 | | 71.174 | 1.00 38.32 |
| ATOM | 9692 | С | LYS | 1431 | | -15.886 | 68.331 | 1.00 33.12 |
| MOTA | 9693 | 0 | LYS | 1431 | | -16.414 | 67.213 | 1.00 32.77 |
| MOTA | 9694 | N | ASN | 1432 | | -16.085 | 69.266 | 1.00 31.72 |
| ATOM | 9695 | CA | ASN | 1432 | | ~16.962 | 69.054 | 1.00 30.83 |
| ATOM | 9696 | CB | ASN | 1432 | | -16.655 | 70.087 | 1.00 29.88 |
| MOTA | 9697 | CG | ASN | 1432 | | -17.463 | 69.860 | 1.00 28.49 |
| MOTA | 9698 | OD1 | | 1432 | | -18.600 | 69.378 | 1.00 27.87 |
| ATOM | 9699 | | ASN | 1432 | | -16.889 | 70.223 | 1.00 26.41 |
| ATOM | 9700 | С | ASN | 1432 | | -18.403 | 69.225 | 1.00 30.31 |
| ATOM | 9701 | 0 | ASN | 1432 | | -18.893 | 70.347 | 1.00 32.09 |
| MOTA | 9702 | N | PHE | 1433 | -6.095 | -19.078 | 68.115 | 1.00 30.31 |
| MOTA | 9703 | CA | PHE | 1433 | | -20.463 | 68.164 | 1.00 30.25 |
| ATOM | 9704 | CB | PHE | 1433 | | -20.840 | 66.878 | 1.00 31.29 |
| ATOM | 9705 | CG | PHE | 1433 | | -20.144 | 66.706 | 1.00 32.82 |
| MOTA | 9706 | CD1 | | 1433 | | -18.899 | 66.095 | 1.00 32.79 |
| ATOM | 9707 | CD2 | | 1433 | | -20.737 | 67.160 | 1.00 33.56 |
| ATOM | 9708 | CE1 | | 1433 | | -18.254 | 65.936 | 1.00 34.13 |
| ATOM | 9709 | CE2 | | 1433 | -11.007 | | 67.007 | 1.00 34.37 |
| ATOM | 9710 | CZ | PHE | 1433 | -11.072 | | 66.394 | 1.00 34.19 |
| ATOM | 9711 | C | PHE | 1433 | | -21.449 | 68.383 | 1.00 30.90 |
| ATOM | 9712 | 0 | PHE | 1433 | | -22.634 | 68.616 | 1.00 30.90 |
| ATOM | 9713 | N | LEU | 1434 | | -20.969 | 68.293 | 1.00 31.92 |
| ATOM | 9714 | CA | LEU | 1434 | | -21.847 | 68.501 | 1.00 33.45 |
| ATOM | 9715 | CB | LEU | 1434 | | -21.276 | 67.834 | 1.00 30.12 |
| ATOM | 9716 | CG | LEU | 1434 | | -22.124 | 67.974 | 1.00 28.48 |
| ATOM | 9717 | | LEU | 1434 | | -23.515 | 67.385 | 1.00 24.04 |
| ATOM | 9718 | CD2 | | 1434 | | -21.422 | 67.263 | 1.00 29.29 |
| ATOM | 9719 | С | LEU | 1434 | | -22.008 | 69.997 | 1.00 35.53 |
| ATOM | 9720 | 0 | LEU | 1434 | | -23.109 | 70.472 | 1.00 35.29 |
| ATOM | 9721 | N | ALA | 1435 | | -20.903 | 70.731 | 1.00 39.10 |
| MOTA | 9722 | CA | ALA | 1435 | | -20.916 | 72.175 | 1.00 43.53 |
| ATOM | 9723 | CB | ALA | 1435 | | -19.512 | 72.741 | 1.00 43.69 |
| ATOM | 9724 | C | ALA | 1435 | | -21.864 | 72.833 | 1.00 46.59 |
| MOTA | 9725 | 0 | ALA | 1435 | | -22.480 | 73.857 | 1.00 48.64 |
| ATOM | 9726 | N | GLU | 1436 | | -21.974 | 72.235 | 1.00 49.35 |
| MOTA | 9727 | CA | GLU | 1436 | | -22.852 | 72.742 | 1.00 52.29 |
| ATOM | 9728 | CB | GLU | 1436 | | -22.507 | 72.085 | 1.00 54.27 |
| ATOM | 9729 | CG | GLU | 1436 | | -21.046 | 72.213 | 1.00 57.48 |
| ATOM | 9730 | CD | GLU | 1436 | -8.111 | -20.674 | 73.617 | 1.00 59.19 |

| MOTA | 9731 | OE1 | GLU | 1436 | -7.296 | -20.800 | 74.557 | 1.00 60.49 |
|------|------|-----|------|------|---------|----------------------|--------|------------|
| MOTA | 9732 | OE2 | GLU | 1436 | -9.278 | -20.251 | 73.779 | 1.00 59.69 |
| ATOM | 9733 | C | GLU | 1436 | | -24.300 | 72.423 | 1.00 52.82 |
| MOTA | 9734 | o | GLU | 1436 | | -25.208 | 72.610 | 1.00 53.16 |
| | 9735 | | | | | | 71.926 | 1.00 53.16 |
| ATOM | | N | THR | 1437 | | -24.504 | | |
| ATOM | 9736 | CA | THR | 1437 | | -25.839 | 71.582 | 1.00 53.71 |
| MOTA | 9737 | CB | THR | 1437 | | -26.343 | 70.268 | 1.00 54.29 |
| MOTA | 9738 | OG1 | THR | 1437 | -4.009 | -27.658 | 69.968 | 1.00 55.02 |
| MOTA | 9739 | CG2 | THR | 1437 | -4.167 | -25.405 | 69.113 | 1.00 55.13 |
| MOTA | 9740 | С | THR | 1437 | -2.332 | -25.849 | 71.440 | 1.00 53.32 |
| ATOM | 9741 | 0 | THR | 1437 | | -25.088 | 72.113 | 1.00 53.43 |
| ATOM | 9742 | N | GLY | 1438 | -1.822 | -26.716 | 70.571 | 1.00 51.53 |
| MOTA | 9743 | CA | GLY | 1438 | | -26.798 | 70.367 | 1.00 49.87 |
| | | | | 1438 | -0.031 | | 68.970 | 1.00 48.04 |
| MOTA | 9744 | C | GLY | | | -27.262 | | |
| MOTA | 9745 | 0 | GLY | 1438 | 1.117 | -27.603 | 68.690 | 1.00 48.97 |
| MOTA | 9746 | N | ASP | 1439 | -1.023 | -27.265 | 68.088 | 1.00 45.31 |
| MOTA | 9747 | CA | ASP | 1439 | -0.826 | -27.699 | 66.714 | 1.00 42.62 |
| MOTA | 9748 | CB | ASP | 1439 | -1.358 | -29.129 | 66.553 | 1.00 44.51 |
| MOTA | 9749 | CG | ASP | 1439 | -1.261 | -29.633 | 65.132 | 1.00 46.55 |
| ATOM | 9750 | OD1 | ASP | 1439 | -2.119 | -29.256 | 64.309 | 1.00 47.77 |
| ATOM | 9751 | OD2 | ASP | 1439 | -0.319 | -30.402 | 64.836 | 1.00 48.59 |
| ATOM | 9752 | C | ASP | 1439 | | -26.747 | 65.758 | 1.00 39.71 |
| ATOM | 9753 | ō | ASP | 1439 | | -26.552 | 65.850 | 1.00 38.19 |
| | 9754 | N | ILE | 1440 | | -26.150 | 64.845 | 1.00 37.29 |
| MOTA | | | | | | | | |
| ATOM | 9755 | CA | ILE | 1440 | | -25.206 | 63.883 | 1.00 34.57 |
| ATOM | 9756 | CB | ILE | 1440 | | -24.751 | 62.861 | 1.00 33.52 |
| ATOM | 9757 | CG2 | ILE | 1440 | -0.920 | | 61.748 | 1.00 33.39 |
| MOTA | 9758 | CG1 | ILE | 1440 | 0.800 | -23.920 ⁻ | 63.572 | 1.00 32.81 |
| ATOM | 9759 | CD1 | ILE | 1440 | 1.930 | -23.460 | 62.678 | 1.00 31.48 |
| ATOM | 9760 | C | ILE | 1440 | -2.540 | -25.774 | 63.138 | 1.00 32.97 |
| ATOM | 9761 | 0 | ILE | 1440 | -3.558 | -25.097 | 62.994 | 1.00 32.77 |
| ATOM | 9762 | N | ARG. | 1441 | | -27.012 | 62.668 | 1.00 31.92 |
| ATOM | 9763 | CA | ARG | 1441 | | -27.631 | 61.947 | 1.00 30.40 |
| ATOM | 9764 | CB | ARG | 1441 | | -28.993 | 61.389 | 1.00 30.10 |
| | | | | | | | | |
| MOTA | 9765 | CG | ARG | 1441 | | -28.897 | 60.205 | 1.00 31.94 |
| MOTA | 9766 | CD | ARG | 1441 | | -30.266 | 59.761 | 1.00 31.51 |
| ATOM | 9767 | NE | ARG | 1441 | | -30.192 | 58.580 | 1.00 31.83 |
| MOTA | 9768 | cz | ARG | 1441 | 0.381 | -29.583 | 58.542 | 1.00 31.78 |
| MOTA | 9769 | NH1 | ARG | 1441 | 0.863 | -28.986 | 59.624 | 1.00 31.49 |
| ATOM | 9770 | NH2 | ARG | 1441 | 1.086 | -29.571 | 57.418 | 1.00 31.50 |
| ATOM | 9771 | С | ARG | 1441 | -4.730 | -27.776 | 62.869 | 1.00 30.29 |
| ATOM | 9772 | O | ARG | 1441 | | -27.702 | 62.432 | 1.00 30.16 |
| ATOM | 9773 | N | ALA | 1442 | | -27.979 | 64.155 | 1.00 29.42 |
| MOTA | 9774 | CA | ALA | 1442 | -5.527 | -28.115 | 65.133 | 1.00 28.31 |
| | | | | | | -28.620 | | 1.00 20.51 |
| MOTA | 9775 | CB | ALA | 1442 | -4.963 | | 66.469 | |
| MOTA | 9776 | C | ALA | 1442 | -6.183 | -26.751 | 65.308 | 1.00 26.62 |
| MOTA | 9777 | 0 | ALA | 1442 | | | 65.471 | 1.00 28.00 |
| MOTA | 9778 | N | ALA | 1443 | -5.377 | -25.694 | 65.270 | 1.00 24.98 |
| MOTA | 9779 | CA | ALA | 1443 | -5.903 | -24.343 | 65.411 | 1.00 24.60 |
| ATOM | 9780 | CB | ALA | 1443 | -4.759 | -23.330 | 65.421 | 1.00 24.64 |
| ATOM | 9781 | C | ALA | 1443 | -6.871 | -24.043 | 64.264 | 1.00 24.55 |
| ATOM | 9782 | 0 | ALA | 1443 | -7.889 | -23.373 | 64.458 | 1.00 24.61 |
| ATOM | 9783 | N | VAL | 1444 | -6 553 | -24.547 | 63.072 | 1.00 24.06 |
| ATOM | 9784 | CA | VAL | 1444 | -7.396 | -24.344 | 61.895 | 1.00 25.36 |
| | 9785 | СВ | VAL | 1444 | | -24.933 | 60.620 | 1.00 25.58 |
| ATOM | | | | 1444 | -7.681 | | 59.430 | 1.00 26.78 |
| ATOM | 9786 | CG1 | | | | -24.782 | | |
| ATOM | 9787 | | VAL | 1444 | -5.423 | -24.217 | 60.338 | 1.00 24.41 |
| ATOM | 9788 | С | VAL | 1444 | -8.757 | -25.002 | 62.086 | 1.00 26.13 |
| MOTA | 9789 | 0 | VAL | 1444 | -9.792 | -24.378 | 61:854 | 1.00 25.38 |
| ATOM | 9790 | N | ARG | 1445 | -8.749 | -26.262 | 62.509 | 1.00 27.76 |
| MOTA | 9791 | CA | ARG | 1445 | -9.988 | -27.001 | 62.723 | 1.00 29.79 |
| MOTA | 9792 | CB | ARG | 1445 | -9.688 | -28.459 | 63.088 | 1.00 30.48 |
| MOTA | 9793 | CG | ARG | 1445 | -9.065 | -29.272 | 61.953 | 1.00 31.74 |
| ATOM | 9794 | CD | ARG | 1445 | -9.068 | -30.766 | 62.259 | 1.00 33.04 |
| ATOM | 9795 | NE | ARG | 1445 | | -31.106 | 63.424 | 1.00 34.02 |
| ATOM | 9796 | CZ | ARG | 1445 | | -31.341 | 63.383 | 1.00 33.14 |
| ATOM | 9797 | | ARG | 1445 | | -31.278 | 62.231 | 1.00 31.44 |
| ATOM | 9798 | | ARG | 1445 | | -31.650 | 64.495 | 1.00 31.44 |
| | | | | | | | | |
| MOTA | 9799 | C | ARG | 1445 | | -26.361 | 63.809 | 1.00 30.41 |
| ATOM | 9800 | 0 | ARG | 1445 | | -26.298 | 63.685 | 1.00 29.87 |
| MOTA | 9801 | N | GLN | 1446 | | -25.877 | 64.868 | 1.00 31.30 |
| MOTA | 9802 | CA | GLN | 1446 | -10.937 | -25.246 | 65.958 | 1.00 32.71 |
| ATOM | 9803 | CB | GLN | 1446 | | -24.877 | 67.098 | 1.00 35.17 |
| ATOM | 9804 | CG | GLN | 1446 | | -24.629 | 68.420 | 1.00 39.56 |
| ATOM | 9805 | CD | GLN | 1446 | -9.759 | -24.160 | 69.514 | 1.00 41.33 |
| MOTA | 9806 | OE1 | GLN | 1446 | -8.609 | -24.608 | 69.599 | 1.00 42.46 |
| MOTA | 9807 | | GLN | 1446 | | -23.262 | 70.371 | 1.00 40.91 |
| | | | | | | | | |

| ATOM | 9808 | С | GLN | 1446 | -11.63 | 32 | -23.988 | 65.440 | 1.00 31.61 |
|--------------|--------------|----------|------------|----------------|--------|----|--------------------|------------------|--------------------------|
| ATOM | 9809 | Ō | GLN | 1446 | | | -23.729 | 65.755 | 1.00 30.44 |
| ATOM | 9810 | N | TYR | 1447 | | | -23.211 | 64.643 | 1.00 31.24 |
| ATOM | 9811 | CA | TYR | 1447 | | | -21.981 | 64.072 | 1.00 30.17 |
| ATOM | 9812 | CB | TYR | 1447 | | | -21.286 | 63.242 | 1.00 29.43 |
| ATOM | 9813 | CG | TYR | 1447 | | | -20.155 | 62.374 | 1.00 28.31 |
| ATOM | 9814 | CD1 | | 1447 | | | -19.059 | 62.927 | 1.00 27.71 |
| ATOM | 9815 | CE1 | TYR | 1447 | | | -18.023 | 62.122 | 1.00 25.98 |
| | 9816 | CD2 | | 1447 | | | -20.190 | 60.990 | 1.00 28.41 |
| ATOM | 9817 | CE2 | TYR | 1447 | | | -19.164 | 60.179 | 1.00 26.24 |
| ATOM | 9818 | CZ | TYR | 1447 | | | -18.087 | 60.748 | 1.00 20.24 |
| ATOM ATOM | 9819 | OH | TYR | 1447 | | | -17.083 | 59.939 | 1.00 26.55 |
| | 9820 | C | TYR | 1447 | | | -22.267 | 63.213 | 1.00 20.55 |
| MOTA | 9821 | | TYR | 1447 | | | -21.559 | 63.301 | 1.00 20.55 |
| ATOM | 9822 | 0 | | | | | -23.309 | 62.392 | 1.00 30.55 |
| ATOM | | N | MET | 1448 1448 | | | -23.702 | 61.521 | 1.00 30.34 |
| MOTA | 9823 | CA | MET MET | 1448 | | | -24.878 | 60.631 | 1.00 30.34 |
| MOTA | 9824 | CB | | | | | -24.529 | | 1.00 30.01 |
| MOTA | 9825 | CG | MET | 1448 | | | -25.991 | 59.580 58.818 | 1.00 31.10 |
| MOTA | 9826 | SD | MET | 1448 | | | | | 1.00 31.00 |
| MOTA | 9827 | CE | MET | 1448 | | | -26.527 | 57.742 | |
| ATOM | 9828 | C | MET | 1448 | | | -24.103 | 62.327 | 1.00 30.96 1.00 29.66 |
| MOTA | 9829 | 0 | MET | 1448 | | | -23.636 | 62.061 | |
| MOTA | 9830 | N | ALA | 1449 | | | -24.976 | 63.308 | 1.00 31.49 |
| MOTA | 9831 | CA | ALA | 1449 | | | -25.467 | 64.152 | 1.00 32.03 1.00 32.34 |
| MOTA | 9832 | CB | ALA | 1449 | | | -26.567 | 65.076 | |
| MOTA | 9833 | C | ALA | 1449 | | | -24.369 | 64.974 | 1.00 32.12 |
| ATOM | 9834 | 0 | ALA | 1449 | | | -24.350 | 65.108 | 1.00 33.68 1.00 32.10 |
| ATOM | 9835 | N | GLU | 1450 | | | -23.460 | 65.529 | |
| ATOM | 9836 | CA | GLU | 1450 | | | -22.382 | 66.335 | 1.00 33.21 1.00 34.06 |
| ATOM | 9837 | CB | GLU | 1450 | | | -21.685 | 67.141 68.353 | 1.00 34.06 |
| MOTA | 9838 | CG CD | GLU | 1450 1450 | | | -22.482 -21.708 | 69.231 | 1.00 38.22 |
| ATOM ATOM | 9839 9840 | | GLU GLU | 1450 | | | -20.539 | 69.549 | 1.00 40.42 |
| ATOM | 9841 | | GLU | 1450 | | | -22.269 | 69.615 | 1.00 41.16 |
| MOTA | 9842 | C | GLU | 1450 | | | -21.359 | 65.508 | 1.00 32.93 |
| ATOM | 9843 | o | GLU | 1450 | | | -20.731 | 66.010 | 1.00 31.71 |
| ATOM | 9844 | N | VAL | 1451 | | | -21.186 | 64.246 | 1.00 31.86 |
| ATOM | 9845 | CA | VAL | 1451 | | | -20.241 | 63.373 | 1.00 31.03 |
| ATOM | 9846 | СВ | VAL | 1451 | | | -19.983 | 62.064 | 1.00 30.01 |
| ATOM | 9847 | | VAL | 1451 | | | -19.275 | 61.041 | 1.00 29.75 |
| ATOM | 9848 | | VAL | | | | -19.133 | 62.367 | 1.00 28.24 |
| ATOM | 9849 | С | VAL | 1451 | -18.73 | 13 | -20.783 | 63.017 | 1.00 31.90 |
| ATOM | 9850 | 0 | VAL | 1451 | -19.70 | 05 | -20.060 | 63.094 | 1.00 32.23 |
| ATOM | 9851 | N | GLU | 1452 | -18.76 | 66 | -22.059 | 62.639 | 1.00 31.88 |
| ATOM | 9852 | CA | GLU | 1452 | -20.03 | 19 | -22.704 | 62.262 | 1.00 33.73 |
| MOTA | 9853 | CB | GLU | 1452 | -19.74 | 41 | -24.083 | 61.660 | 1.00 34.97 |
| MOTA | 9854 | CG | GLU | 1452 | -20.99 | 93 | -24.838 | 61.243 | 1.00 38.84 |
| MOTA | 9855 | CD | GLU | 1452 | | | -26.118 | 60.490 | 1.00 41.04 |
| MOTA | 9856 | | GLU | 1452 | | | -26.820 | 60.088 | 1.00 42.35 |
| MOTA | 9857 | OE2 | GLU | 1452 | | | -26.421 | 60.296 | 1.00 43.66 |
| ATOM | 9858 | С | GLU | 1452 | | | -22.846 | 63.444 | 1.00 34.26 |
| MOTA | 9859 | 0 | GLU | 1452 | | | -22.815 | 63.274 | 1.00 33.56 |
| MOTA | 9860 | N | SER | 1453 | | | -22.996 | 64.638 | 1.00 34.47 |
| ATOM | 9861 | CA | SER | 1453 | | | -23.145 | 65.850 | 1.00 35.91 |
| ATOM | 9862 | CB | SER | 1453 | | | -23.918 | 66.903 | 1.00 36.48 |
| ATOM | 9863 | OG | SER | 1453 | -20.06 | | -25.205 | 66.416 | 1.00 39.52 |
| MOTA | 9864 | С | SER | 1453 | -21.60 | | -21.786 | 66.414 | 1.00 35.30 |
| ATOM | 9865 | 0 | SER | 1453 | | | -21.690 | 67.269 | 1.00 35.49 |
| ATOM | 9866 | N | GLY | 1454 | -20.95 | | -20.737 | 65.929 | 1.00 33.14 |
| ATOM | 9867 | CA | GLY | 1454 | | | -19.405 | 66.407 67.624 | 1.00 32.40 1.00 31.91 |
| ATOM | 9868 9869 | С 0 | GLY GLY | $1454 \\ 1454$ | | | -19.042 -17.906 | 68.100 | 1.00 31.31 |
| ATOM ATOM | 9870 | N | VAL | 1455 | | | -20.008 | 68.132 | 1.00 32.10 |
| ATOM | 9871 | CA | VAL | 1455 | | | -19.781 | 69.298 | 1.00 31.24 |
| ATOM | 9872 | CB | VAL | 1455 | | | -21.009 | 69.580 | 1.00 31.24 |
| ATOM | 9873 | | VAL | 1455 | | | -20.735 | 70.777 | 1.00 32.33 |
| MOTA | 9874 | | VAL | 1455 | | | -22.241 | 69.820 | 1.00 33.67 |
| ATOM | 9875 | C | VAL | 1455 | | | -18.570 | 69.033 | 1.00 30.78 |
| ATOM | 9876 | ō | VAL | 1455 | | | -17.722 | 69.905 | 1.00 30.55 |
| ATOM | 9877 | N | TYR | 1456 | | | -18.500 | 67.815 | 1.00 28.80 |
| ATOM | 9878 | CA | TYR | 1456 | | | -17.401 | 67.405 | 1.00 27.94 |
| ATOM | 9879 | CB | TYR | 1456 | | | -17.935 | 67.012 | 1.00 26.12 |
| ATOM | 9880 | CG | TYR | 1456 | | | -16.846 | 66.531 | 1.00 23.34 |
| ATOM | 9881 | CD1 | TYR | 1456 | | | -15.950 | 67.433 | 1.00 22.92 |
| MOTA | 9882 | CE1 | TYR | 1456 | -12.87 | 73 | -14.883 | 66.995 | 1.00 22.74 |
| MOTA | 9883 | CD2 | TYR | 1456 | -13.98 | 39 | -16.652 | 65.169 | 1.00 24.91 |
| MOTA | 9884 | CE2 | TYR | 1456 | -13.23 | 12 | -15.585 | 64.718 | 1.00 22.93 |

| ATOM | 9885 | CZ | TYR | 1456 | -12.663 | -14.704 | 65.634 | 1.00 23.92 |
|------|------|-----|-----|-------|---------|---------|--------|-------------|
| ATOM | 9886 | ОН | TYR | 1456 | | -13.618 | 65.204 | 1.00 24.81 |
| | 9887 | C | TYR | 1456 | | -16.671 | 66.208 | 1.00 27.24 |
| MOTA | | | | | | | | |
| MOTA | 9888 | 0 | TYR | 1456 | | -17.308 | 65.259 | 1.00 27.22 |
| MOTA | 9889 | N | PRO | 1457 | -17.178 | -15.328 | 66.242 | 1.00 28.94 |
| MOTA | 9890 | CD | PRO | 1457 | -17.470 | -14.508 | 65.053 | 1.00 28.55 |
| ATOM | 9891 | CA | PRO | 1457 | -16.660 | -14.494 | 67.331 | 1.00 29.57 |
| ATOM | 9892 | СВ | PRO | 1457 | | -13.167 | 66.638 | 1.00 29.55 |
| | | | | | | | | |
| MOTA | 9893 | CG | PRO | 1457 | | -13.105 | 65.607 | 1.00 31.60 |
| MOTA | 9894 | С | PRO | 1457 | -17.634 | -14.338 | 68.499 | 1.00 31.24 |
| MOTA | 9895 | 0 | PRO | 1457 | -18.850 | -14.454 | 68:333 | 1.00 31.53 |
| ATOM | 9896 | N | GLY | 1458 | -17.085 | -14.081 | 69.683 | 1.00 32.29 |
| ATOM | 9897 | CA | GLY | 1458 | | -13.903 | 70.864 | 1.00 33.07 |
| | 9898 | C | GLY | 1458 | | -12.429 | 71.129 | 1.00 34.59 |
| ATOM | | | | | | | | |
| ATOM | 9899 | 0 | GLY | 1458 | | -11.583 | 70.431 | 1.00 34.41 |
| MOTA | 9900 | N | GLU | 1459 | -18.931 | -12.106 | 72.135 | 1.00 34.02 |
| MOTA | 9901 | CA | GLU | 1459 | -19.191 | -10.711 | 72.447 | 1.00 35.57 |
| ATOM | 9902 | CB | GLU | 1459 | -20.174 | -10.591 | 73.616 | 1.00 39.24 |
| ATOM | 9903 | CG | GLU | 1459 | -21.239 | -9.530 | 73.394 | 1.00 41.27 |
| ATOM | 9904 | CD | GLU | 1459 | -22.226 | -9.926 | 72.309 | 1.00 42.55 |
| | | | | | | | | |
| MOTA | 9905 | OE1 | | 1459 | -22.962 | -9.046 | 71.815 | 1.00 43.59 |
| MOTA | 9906 | OE2 | GLU | 1459 | -22.272 | -11.123 | 71.954 | 1.00 44.59 |
| MOTA | 9907 | C | GLU | 1459 | -17.886 | -10.004 | 72.798 | 1.00 34.39 |
| MOTA | 9908 | 0 | GLU | -1459 | -17.763 | -8.790 | 72.634 | 1.00 34.39 |
| ATOM | 9909 | N | GLU | 1460 | | -10.775 | 73.271 | 1.00 33.94 |
| | 9910 | | | | | -10.232 | 73.645 | 1.00 34.54 |
| MOTA | | CA | GLU | 1460 | | | | |
| ATOM | 9911 | CB | GLŲ | 1460 | | -11.277 | 74.404 | 1.00 37.12 |
| MOTA | 9912 | CG | GLU | 1,460 | -15.592 | -12.160 | 75.331 | 1.00 41.64 |
| ATOM | 9913 | CD | GLU | 1460 | -16.379 | -13.213 | 74.579 | 1.00 43.05 |
| MOTA | 9914 | OE1 | GLU | 1460 | -15.745 | -14.100 | 73.961 | 1.00 43.71 |
| ATOM | 9915 | OE2 | | 1460 | | -13.148 | 74.600 | 1.00 44.97 |
| | | | | | | | | |
| MOTA | 9916 | С | GLU | 1460 | -14.828 | -9.816 | 72.404 | 1.00 33.32 |
| MOTA | 9917 | 0 | GLU | 1460 | -13.883 | -9.031 | 72.488 | 1.00 33.42 |
| MOTA | 9918 | N | HIS | 1461 | -15.227 | -10.358 | 71.258 | 1.00 31.67 |
| MOTA | 9919 | CA | HIS | 1461 | -14.571 | -10.067 | 69.986 | 1.00 30.54 |
| MOTA | 9920 | CB | HIS | 1461 | -14.304 | -11.368 | 69.224 | 1.00 30.83 |
| ATOM | 9921 | CG | HIS | 1461 | | -12.382 | 70.002 | 1.00 30.96 |
| | | | | | | | | |
| MOTA | 9922 | | HIS | 1461 | -13.853 | -13.630 | 70.415 | 1.00 30.87 |
| MOTA | 9923 | | HIS | 1461 | | -12.160 | 70.433 | 1.00 31.51 |
| MOTA | 9924 | CE1 | HIS | 1461 | -11.800 | -13.228 | 71.077 | 1.00 32.78 |
| MOTA | 9925 | NE2 | HIS | 1461 | -12.761 | -14.134 | 71.080 | 1.00 30.95 |
| MOTA | 9926 | С | HIS | 1461 | -15.443 | -9.169 | 69.121 | 1.00 30.10 |
| ATOM | 9927 | ō | HIS | 1461 | -15.096 | -8.871 | 67.979 | 1.00 28.36 |
| | | | | | | | | |
| ATOM | 9928 | N | SER | 1462 | -16.573 | -8.742 | 69.677 | 1.00 29.88 |
| ATOM | 9929 | CA | SER | 1462 | -17.526 | -7.901 | 68.962 | 1.00 31.52 |
| ATOM | 9930 | CB | SER | 1462 | -18.930 | -8.484 | 69.111 | 1.00 29.18 |
| MOTA | 9931 | OG | SER | 1462 | -18.956 | -9.846 | 68.726 | 1.00 31.95 |
| ATOM | 9932 | С | SER | 1462 | -17.538 | -6.453 | 69.440 | 1.00 33.19 |
| ATOM | 9933 | ō | SER | 1462 | -17.161 | -6.161 | 70.576 | 1.00 33.68 |
| | | | | | -17.981 | -5.550 | 68.567 | 1.00 33.32 |
| MOTA | 9934 | N | PHE | 1463 | | | | |
| MOTA | 9935 | CA | PHE | 1463 | -18.057 | -4.130 | 68.900 | 1.00 34.66 |
| MOTA | 9936 | CB | PHE | 1463 | -17.364 | -3.274 | 67.834 | 1.00 35.23 |
| ATOM | 9937 | CG. | PHE | 1463 | -15.895 | -3.555 | 67.684 | 1.00 36.25 |
| ATOM | 9938 | | PHE | 1463 | -15.453 | -4.650 | 66.951 | 1.00 36.98 |
| ATOM | 9939 | | PHE | 1463 | -14.952 | -2.721 | 68.278 | 1.00 37.01 |
| ATOM | 9940 | | PHE | 1463 | -14.092 | -4.910 | 66.807 | 1.00 37.76 |
| | | | | | | | 68.142 | 1.00 37.70 |
| ATOM | 9941 | | PHE | 1463 | -13.587 | -2.971 | | |
| MOTA | 9942 | CZ | PHE | 1463 | -13.157 | -4.068 | 67.405 | 1.00 37.03 |
| ATOM | 9943 | С | PHE | 1463 | -19.513 | -3.685 | 69.027 | 1.00 35.85 |
| ATOM | 9944 | 0 | PHE | 1463 | -20.420 | -4.319 | 68.486 | 1.00 33.90 |
| ATOM | 9945 | N | HIS | 1464 | -19.727 | -2.585 | 69.740 | 1.00 37.39 |
| | 9946 | CA | HIS | 1464 | -21.068 | -2.053 | 69.949 | 1.00 39.80 |
| ATOM | | | | | -21.623 | | | 1.00 39.63 |
| ATOM | 9947 | CB | HIS | 1464 | | -2.538 | 71.289 | |
| ATOM | 9948 | CG | HIS | 1464 | -21.853 | -4.016 | 71.342 | 1.00 40.65 |
| ATOM | 9949 | | HIS | 1464 | -21.226 | -4.995 | 72.038 | 1.00 40.98 |
| ATOM | 9950 | ND1 | HIS | 1464 | -22.818 | -4.644 | 70.585 | 1.00 39.94 |
| ATOM | 9951 | | HIS | 1464 | -22.776 | -5.945 | 70.810 | 1.00 40.36 |
| ATOM | 9952 | MES | HIS | 1464 | -21.818 | -6.185 | 71.688 | 1.00 40.96 |
| | | | | | | | | |
| ATOM | 9953 | C | HIS | 1464 | -21.042 | -0.535 | 69.920 | 1.00 40.95 |
| ATOM | 9954 | 0 | HIS | 1464 | -21.911 | 0.059 | 69.243 | 1.00 41.98 |
| MOTA | 9955 | OXT | HIS | 1464 | -20.156 | 0.038 | 70.583 | 1.00 42.55. |
| ATOM | 9956 | C1 | KPL | 1465 | -8.662 | -8.598 | 56.997 | 1.00 40.66 |
| ATOM | 9957 | C2 | KPL | 1465 | -9.406 | -8.731 | 55.651 | 1.00 40.02 |
| ATOM | 9958 | C3 | KPL | 1465 | -9.470 | -10.212 | 55.264 | 1.00 40.28 |
| | | | | | -10.847 | -8.205 | 55.810 | 1.00 40.20 |
| ATOM | 9959 | C4 | KPL | 1465 | | | | |
| ATOM | 9960 | 01 | KPL | 1465 | -10.844 | -6.822 | 56.181 | 1.00 43.78 |
| MOTA | 9961 | C5 | KPL | 1465 | -8.646 | -7.947 | 54.549 | 1.00 38.37 |
| | | | | | | | | |

| MOTA | 9962 | 02 | KPL | 1465 | -9.203 | -7.052 | 53.945 | 1.00 | 39.08 |
|------|-------|-----|-----|------|--------|---------|--------|------|----------------|
| ATOM | 9963 | C6 | KPL | 1465 | -7.208 | -8.268 | 54.193 | 1.00 | 36.59 |
| ATOM | 9964 | 03 | KPL | 1465 | -6.611 | -9.157 | 54.768 | 1.00 | 34.92 |
| ATOM | 9965 | 04 | KPL | 1465 | -6.578 | -7.561 | 53.231 | | 31.35 |
| ATOM | 9966 | CB | MET | 1501 | 12.451 | -25.585 | -6.577 | | 68.45 |
| | 9967 | CG | MET | 1501 | 12.983 | -25.086 | -7.922 | | 70.78 |
| ATOM | | | | | | | | | 73.21 |
| ATOM | 9968 | SD | MET | 1501 | 14.555 | -25.814 | -8.446 | ** | |
| ATOM | 9969 | CE | MET | 1501 | 15.640 | -24.379 | -8.381 | | 72.59 |
| MOTA | 9970 | С | MET | 1501 | | -26.660 | -5.175 | | 64.43 |
| ATOM | 9971 | 0 | MET | 1501 | 13.933 | -27.714 | -5.740 | | 64.33 |
| ATOM | 9972 | N | MET | 1501 | 14.252 | -24.188 | -5.606 | 1.00 | 67.20 |
| MOTA | 9973 | CA | MET | 1501 | 13.404 | -25.395 | -5.390 | 1.00 | 66.44 |
| ATOM | 9974 | N | LYS | 1502 | 15.270 | -26.551 | -4.351 | 1.00 | 61.82 |
| ATOM | 9975 | CA | LYS | 1502 | 16.137 | -27.690 | -4.067 | 1.00 | 58.51 |
| ATOM | 9976 | СВ | LYS | 1502 | 17.506 | -27.493 | -4.719 | | 59.36 |
| MOTA | 9977 | CG | LYS | 1502 | 17.454 | -27.205 | -6.219 | | 59.84 |
| | 9978 | CD | LYS | 1502 | 16.747 | -28.314 | -6.992 | | 60.21 |
| ATOM | | | | | | | -6.871 | 1.00 | |
| ATOM | 9979 | CE | LYS | 1502 | | -29.641 | | | |
| MOTA | 9980 | NZ | LYS | 1502 | | -30.731 | -7.593 | | 60.90 |
| MOTA | 9981 | С | LYS | 1502 | | -27.938 | -2.562 | 1.00 | |
| MOTA | 9982 | 0 | LYS | 1502 | 16.023 | -29.039 | -2.083 | 1.00 | 56.98 |
| MOTA | 9983 | N | PRO | 1503 | 16.733 | -26.918 | -1.795 | | 51.21 |
| ATOM | 9984 | CD | PRO | 1503 | 16.674 | -27.002 | -0.323 | 1.00 | 49.69 |
| ATOM | 9985 | CA | PRO | 1503 | 17.082 | -25.554 | -2.213 | 1.00 | 46.71 |
| ATOM | 9986 | CB | PRO | 1503 | 16.764 | -24.739 | -0.973 | 1.00 | 48.28 |
| ATOM | 9987 | CG | PRO | 1503 | | -25.653 | 0.112 | | 49.41 |
| ATOM | 9988 | C | PRO | 1503 | | 25.434 | -2.610 | | 42.37 |
| | 9989 | | PRO | 1503 | | -26.369 | -2.433 | | 41.84 |
| ATOM | | | | | | -24.274 | -3.142 | | 37.50 |
| ATOM | 9990 | N | THR | 1504 | | | | | |
| ATOM | 9991 | CA | THR | 1504 | | -24.024 | -3.565 | | 33.10 |
| ATOM | 9992 | CB | THR | 1504 | 20.375 | -22.784 | -4.485 | | 32.53 |
| ATOM | 9993 | OG1 | THR | 1504 | 19.578 | -23.011 | -5.653 | | 33.15 |
| MOTA | 9994 | CG2 | THR | 1504 | 21.808 | -22.502 | -4.905 | 1.00 | 29.59 |
| MOTA | 9995 | С | THR | 1504 | 21.190 | -23.805 | -2.342 | 1.00 | 31.99 |
| MOTA | 9996 | 0 | THR | 1504 | 20.826 | -23.069 | -1.425 | 1.00 | 29.30 |
| ATOM | 9997 | N | THR | 1505 | 22.354 | -24.446 | -2.332 | 1.00 | 30.78 |
| ATOM | 9998 | CA | THR | 1505 | 23.273 | -24.324 | -1.208 | 1.00 | 29.63 |
| ATOM | 9999 | СВ | THR | 1505 | 23.305 | -25.619 | -0.369 | | 29:85 |
| ATOM | 10000 | OG1 | THR | 1505 | | -26.674 | -1.138 | | 31.33 |
| | | | | 1505 | | -26.029 | 0.036 | | 29.10 |
| ATOM | 10001 | CG2 | THR | | | | | | 29.48 |
| ATOM | 10002 | C | THR | 1505 | | -24.014 | -1.659 | | |
| ATOM | 10003 | 0 | THR | 1505 | | -24.056 | -2.850 | | 27.82 |
| MOTA | 10004 | N | ILE | 1506 | 25.557 | -23.708 | -0.693 | | 29.78 |
| ATOM | 10005 | CA | ILE | 1506 | 26.950 | -23.391 | -0.975 | | 30.15 |
| MOTA | 10006 | CB | ILE | 1506 | 27.723 | -23.108 | 0.331 | 1.00 | 31.02 |
| MOTA | 10007 | CG2 | ILE | 1506 | 29.122 | -22.597 | 0.013 | 1.00 | 30.67 |
| MOTA | 10008 | CG1 | ILE | 1506 | 26.966 | -22.065 | 1.161 | 1.00 | 31.55 |
| ATOM | 10009 | CD1 | ILE | 1506 | 27.492 | -21.896 | 2.576 | 1.00 | 33.42 |
| ATOM | 10010 | С | ILE | 1506 | 27.593 | -24.568 | -1.705 | 1.00 | 30.17 |
| ATOM | 10011 | ō | ILE | 1506 | 28.525 | -24.394 | -2.491 | | 30.44 |
| ATOM | 10012 | N | SER | 1507 | 27.077 | -25.765 | -1.441 | | 31.25 |
| ATOM | | CA | SER | 1507 | | -26.990 | -2.059 | | 33.43 |
| | 10013 | | | | | -28.180 | -1.646 | | 34.53 |
| ATOM | 10014 | CB | SER | 1507 | | | | | |
| MOTA | 10015 | OG | SER | 1507 | | -28.258 | -0.238 | | 39.65 33.68 |
| ATOM | 10016 | С | SER | 1507 | | -26.889 | -3.580 | | |
| ATOM | 10017 | 0 | SER | 1507 | 28.551 | -27.269 | -4.234 | | 33.38 |
| ATOM | 10018 | N | LEU | 1508 | 26.483 | -26.383 | -4.137 | | 32.89 |
| MOTA | 10019 | CA | LEU | 1508 | 26.361 | -26.242 | -5.582 | | 32.80 |
| ATOM | 10020 | CB | LEU | 1508 | 24.970 | -25.720 | -5.958 | 1.00 | 34.32 |
| ATOM | 10021 | CG | LEU | 1508 | 24.031 | -26.678 | -6.701 | 1.00 | 36.26 |
| ATOM | 10022 | CD1 | LEU | 1508 | 22.694 | -25.992 | -6.951 | 1.00 | 36.00 |
| ATOM | 10023 | CD2 | LEU | 1508 | 24.661 | -27.114 | -8.009 | 1.00 | 36.33 |
| ATOM | 10024 | C | LEU | 1508 | | -25.307 | -6.156 | | 31.90 |
| ATOM | 10025 | o | LEU | 1508 | | -25.597 | -7.196 | | 32.06 |
| | 10025 | | LEU | 1509 | | -24.187 | -5.482 | | 29.72 |
| ATOM | | N | | 1509 | | | | | 29.54 |
| ATOM | 10027 | CA | LEU | | | -23.226 | -5.959 | | |
| ATOM | 10028 | CB | LEU | 1509 | | -21.946 | -5.116 | | 29.54 |
| ATOM | 10029 | CG | LEU | 1509 | 27.233 | -21.237 | -5.105 | | 29.15 |
| ATOM | 10030 | CD1 | LEU | 1509 | | -19.898 | -4.383 | | 30.33 |
| ATOM | 10031 | CD2 | LEU | 1509 | | -21.021 | -6.535 | | 28.87 |
| ATOM | 10032 | С | LEU | 1509 | 30.044 | -23.830 | -5.927 | | 30.18 |
| ATOM | 10033 | 0 | LEU | 1509 | 30.875 | -23.559 | -6.799 | 1.00 | 27.72 |
| ATOM | 10034 | N | GLN | 1510 | | -24.658 | -4.920 | 1.00 | 30.60 |
| ATOM | 10035 | CA | GLN | 1510 | | -25.308 | -4.779 | | 32.89 |
| ATOM | 10036 | CB | GLN | 1510 | | -26.008 | -3.419 | | 32.23 |
| MOTA | 10037 | CG | GLN | 1510 | | -26.521 | -3.051 | | 34.03 |
| | | | | | | -25.452 | -3.146 | | 35.52 |
| ATOM | 10038 | CD | GLN | 1510 | 74.17/ | 20.402 | -2.14O | 1.00 | 22.22 |

| ATOM | 10039 | OE1 | GLN | 1510 | 34.673 | -25.187 | -4.223 | 1.00 36.22 |
|------|-------|-----|-------|-------|--------|---------|---------|------------|
| ATOM | 10040 | NE2 | GLN | 1510 | 34.452 | -24.824 | -2.017 | 1.00 34.94 |
| ATOM | 10041 | С | GLN | 1510 | | -26.312 | -5.920 | 1.00 33.79 |
| ATOM | 10042 | ō | GLN | 1510 | 32.852 | -26.537 | -6.408 | 1.00 34.78 |
| | 10042 | N | LYS | 1511 | | -26.906 | -6.345 | 1.00 35.14 |
| MOTA | | | | | | | | |
| MOTA | 10044 | CA | LYS | 1511 | 30.659 | | -7.446 | 1.00 36.98 |
| MOTA | 10045 | CB | LYS | 1511 | 29.309 | -28.574 | -7.574 | 1.00 38.13 |
| MOTA | 10046 | CG | LYS | 1511 | | -29.386 | -8.859 | 1.00 40.56 |
| ATOM | 10047 | CD | LYS | 1511 | 27.711 | -29.594 | -9.259 | 1.00 43.87 |
| MOTA | 10048 | CE | LYS | 1511 | 26.973 | -30.517 | -8.299 | 1.00 45.00 |
| ATOM | 10049 | NZ | LYS | 1511 | 25.536 | -30.670 | -8.686 | 1.00 47.90 |
| MOTA | 10050 | С | LYS | 1511 | 30.955 | -27.127 | -8.750 | 1.00 36.69 |
| ATOM | 10051 | 0 | LYS | 1511 | 31.694 | -27.619 | -9.599 | 1.00 37.22 |
| ATOM | 10052 | N | TYR | 1512 | 30.371 | | -8.899 | 1.00 36.54 |
| ATOM | 10053 | CA | TYR | 1512 | 30.560 | -25.141 | | 1.00 35.65 |
| ATOM | 10053 | CB | TYR | 1512 | | -23.900 | | 1.00 37.28 |
| | | | | | | | | |
| MOTA | 10055 | CG | TYR | 1512 | | -24.188 | | 1.00 39.20 |
| MOTA | 10056 | CD1 | TYR | 1512 | | -23.175 | | 1.00 41.06 |
| ATOM | 10057 | CE1 | TYR | 1512 | | -23.429 | | 1.00 42.03 |
| MOTA | 10058 | CD2 | TYR | 1512 | | -25.468 | | 1.00 40.61 |
| MOTA | 10059 | CE2 | TYR | 1512 | 26.382 | -25.734 | -10.673 | 1.00 41.29 |
| MOTA | 10060 | CZ | TYR | 1512 | 25.463 | -24.710 | -10.506 | 1.00 42.07 |
| ATOM | 10061 | OH | TYR | 1512 | 24.117 | -24.963 | -10.646 | 1.00 43.50 |
| ATOM | 10062 | С | TYR | 1512 | | -24.716 | | 1.00 36.33 |
| ATOM | 10063 | 0 | TYR | 1512 | | -24.771 | | 1.00 34.44 |
| ATOM | 10064 | N | LYS | 1513 | | -24.277 | -9.274 | 1.00 35.91 |
| ATOM | 10065 | CA | LYS | 1513 | | -23.858 | -9.426 | 1.00 37.24 |
| | | | | 1513 | | -23.362 | -8.090 | 1.00 37.24 |
| MOTA | 10066 | CB | LÝS | | | | | |
| ATOM | 10067 | CG | LYS | 1513 | | -23.108 | -8.136 | 1.00 32.35 |
| MOTA | 10068 | CD | LYS | 1513 | | -22.091 | -7.096 | 1.00 31.84 |
| ATOM | 10069 | CE | LYS | 1513 | | -21.848 | -7.198 | 1.00 30.35 |
| ATOM | 10070 | NZ | LYS- | 1513 | 38.524 | -20.591 | -6.529 | 1.00 29.60 |
| MOTA | 10071 | C | LYS | 1513 | 34.907 | -25.022 | -9.954 | 1.00 38.69 |
| ATOM | 10072 | 0 | LYS | 1513 | 35.870 | -24.829 | -10.694 | 1.00 39.24 |
| ATOM | 10073 | N | GLN | 1514 | 34.517 | -26.231 | -9.567 | 1.00 40.67 |
| ATOM | 10074 | CA | GLN | 1514 | 35.205 | -27.437 | -9.995 | 1.00 43.38 |
| ATOM | 10075 | СВ | GLN | 1514 | | -28.623 | -9.160 | 1.00 45.15 |
| ATOM | 10076 | CG | GLN | 1514 | | -28.565 | -7.710 | 1.00 48.35 |
| ATOM | 10070 | CD | GLN | 1514 | 34.481 | | -6.855 | 1.00 49.83 |
| | | | | | | | | |
| ATOM | 10078 | | GLN | 1514 | | -30.669 | -7.343 | 1.00 51.33 |
| MOTA | 10079 | NE2 | | 1514 | 34.321 | | -5.570 | 1.00 50.47 |
| MOTA | 10080 | С | GLN | 1514 | | -27.704 | | 1.00 43.74 |
| ATOM | 10081 | 0 | GLN | 1514 | | -28.148 | | 1.00 44.54 |
| ATOM | 10082 | N | GLU . | 1515. | | -27.428 | | 1.00 43.52 |
| ATOM | 10083 | CA | GLU | 1515 | 33.329 | -27.637 | -13.291 | 1.00 43.19 |
| ATOM | 10084 | CB | GLU | 1515 | 31.830 | -27.920 | -13.394 | 1.00 44.57 |
| ATOM | 10085 | ·CG | GLU | 1515 | 31.351 | -29.051 | -12.502 | 1.00 46.62 |
| ATOM | 10086 | CD | GLU | 1515 | | -29.430 | | 1.00 48.59 |
| ATOM | 10087 | | GLU | 1515 | | -28.525 | | 1.00 48.92 |
| ATOM | 10088 | OE2 | | 1515 | | -30.637 | | 1.00 51.45 |
| ATOM | 10089 | C | GLU | 1515 | | -26.417 | | 1.00 42.44 |
| | | | | | | | | 1.00 42.44 |
| ATOM | 10090 | 0 | | | + | | | |
| ATOM | 10091 | N | LYS | 1516 | | -25.405 | | 1.00 40.37 |
| MOTA | 10092 | CA | LYS | 1516 | | -24.169 | | 1.00 39.50 |
| ATOM | 10093 | СВ | LYS | 1516 | | -24.459 | | 1.00 40.90 |
| ATOM | 10094 | CG | LYS | 1516 | | -25.031 | | 1.00 42.75 |
| MOTA | 10095 | CD | LYS | 1516 | 37.714 | -24.039 | -13.919 | 1.00 45.19 |
| MOTA | 10096 | CE | LYS | 1516 | 39.074 | -24.585 | -13.498 | 1.00 46.49 |
| ATOM | 10097 | NZ | LYS | 1516 | 39.950 | -24.871 | -14.670 | 1.00 48.49 |
| MOTA | 10098 | С | LYS | 1516 | 33.408 | -23.475 | -14.768 | 1.00 38.14 |
| ATOM | 10099 | 0 | LYS | 1516 | 33.512 | -22.731 | -15.745 | 1.00 38.51 |
| ATOM | 10100 | N | LYS | 1517 | | -23.727 | | 1.00 35.26 |
| ATOM | 10101 | CA | LYS | .1517 | | -23.128 | | 1.00 33.69 |
| | | | | | | -24.084 | | 1.00 34.32 |
| ATOM | 10102 | CB | LYS | 1517 | | -24.084 | | 1.00 34.32 |
| ATOM | 10103 | CG | LYS | 1517 | | | | |
| ATOM | 10104 | CD | LYS | 1517 | | -24.446 | | 1.00 37.44 |
| MOTA | 10105 | CE | LYS | 1517 | | -25.896 | | 1.00 39.19 |
| MOTA | 10106 | NZ | LYS | 1517 | | -26.777 | | 1.00 41.39 |
| MOTA | 10107 | C | LYS | 1517 | 30.765 | -21.823 | -13.878 | 1.00 31.87 |
| MOTA | 10108 | 0 | LYS | 1517 | 30.366 | -21.830 | -12.715 | 1.00 31.03 |
| MOTA | 10109 | N | ARG | 1518 | | -20.704 | | 1.00 30.53 |
| MOTA | 10110 | CA | ARG | 1518 | | -19.399 | | 1.00 28.43 |
| ATOM | 10111 | СВ | ARG | 1518 | | -18.319 | | 1.00 30.06 |
| MOTA | 10112 | CG | ARG | 1518 | | -18.306 | | 1.00 31.46 |
| ATOM | 10112 | CD | ARG | 1518 | | -17.421 | | 1.00 33.23 |
| ATOM | 10113 | | ARG. | 1518 | | -18.071 | | 1.00 35.53 |
| | | NE | | | | -17.523 | | 1.00 35.33 |
| MOTA | 10115 | cz | ARG | 1518 | 34.134 | 11.343 | 10.103 | 1.00 30.40 |

| ATOM | 10116 | NH1 | ARG | 1518 | 34.723 | -16.308 | -18.113 | 1.00 34.15 |
|------|-------|-----|-----|------|--------|---------|---------|------------|
| ATOM | | | ARG | 1518 | | -18.194 | | 1.00 37.73 |
| ATOM | | C | ARG | 1518 | | -19.127 | | 1.00 27.86 |
| ATOM | | Õ | ARG | 1518 | | -19.234 | | 1.00 27.30 |
| | | N | PHE | 1519 | | -18.776 | | 1.00 25.52 |
| ATOM | | | | | | | | 1.00 23.32 |
| ATOM | | CA | PHE | 1519 | | -18.518 | | |
| ATOM | | CB | PHE | 1519 | | -19.382 | | 1.00 23.24 |
| ATOM | | CG | PHE | 1519 | | -19.109 | -9.646 | 1.00 22.05 |
| ATOM | 10124 | | PHE | 1519 | | -18.085 | -8.755 | 1.00 22.20 |
| ATOM | 10125 | CD2 | PHE | 1519 | 29.311 | -19.851 | -9.428 | 1.00 24.57 |
| ATOM | 10126 | CE1 | PHE | 1519 | 28.650 | -17.800 | -7.666 | 1.00 20.88 |
| ATOM | 10127 | CE2 | PHE | 1519 | 30.142 | -19.575 | -8.342 | 1.00 24.45 |
| ATOM | 10128 | CZ | PHE | 1519 | 29.810 | -18.547 | -7.457 | 1.00 23.26 |
| ATOM | | С | PHE | 1519 | | -17.048 | -11.738 | 1.00 23.05 |
| АТОМ | | ō | PHE | 1519 | | -16.314 | | 1.00 21.97 |
| ATOM | | N | ALA | 1520 | | -16.627 | | 1.00 21.46 |
| ATOM | | CA | ALA | 1520 | | -15.250 | | 1.00 20.80 |
| | | | | | | | | |
| ATOM | | CB | ALA | 1520 | | -14.747 | | 1.00 20.77 |
| MOTA | | С | ALA | 1520 | | -15.098 | | 1.00 19.62 |
| ATOM | | 0 | ALA | 1520 | | -15.980 | -9.936 | 1.00 20.43 |
| MOTA | | N | THR | 1521 | | -13.972 | -9.688 | 1.00 19.21 |
| ATOM | 10137 | CA | THR | 1521 | 24.602 | -13.663 | -8.406 | 1.00 20.28 |
| ATOM | 10138 | CB | THR | 1521 | 25.626 | -13.736 | -7.259 | 1.00 20.78 |
| MOTA | 10139 | OG1 | THR | 1521 | 26.154 | -15.070 | -7.183 | 1.00 23.74 |
| ATOM | 10140 | CG2 | THR | 1521 | 24.967 | -13.386 | -5.934 | 1.00 27.16 |
| ATOM | | С | THR | 1521 | 24.030 | -12.250 | -8.495 | 1.00 17.98 |
| АТОМ | | ō | THR | 1521 | | -11.435 | -9.300 | 1.00 17.51 |
| ATOM | | N | ILE | 1522 | | -11.942 | -7.666 | 1.00 17.55 |
| ATOM | | CA | ILE | 1522 | | -10.626 | -7.746 | 1.00 15.48 |
| | | CB | ILE | | | | -8.726 | 1.00 15.40 |
| ATOM | | | | 1522 | | -10.684 | | |
| ATOM | | CG2 | | 1522 | | -11.381 | -8.064 | 1.00 15.09 |
| ATOM | | CG1 | | 1522 | 20.846 | -9.276 | -9.185 | 1.00 15.40 |
| ATOM | 10148 | | ILE | 1522 | 21.865 | | -10.104 | 1.00 21.34 |
| ATOM | | С | ILE | 1522 | | -10.131 | -6.386 | 1.00 15.61 |
| ATOM | 10150 | 0 | ILE | 1522 | 21.694 | -10.926 | -5.485 | 1.00 13.97 |
| ATOM | 10151 | N | THR | 1523 | 21.825 | -8.818 | -6.226 | 1.00 17.24 |
| ATOM | 10152 | CA | THR | 1523 | 21.331 | -8.289 | -4.962 | 1.00 16.39 |
| ATOM | 10153 | CB | THR | 1523 | 21.855 | -6.859 | -4.657 | 1.00 16.96 |
| ATOM | | OG1 | THR | 1523 | 21.353 | -5.938 | -5.628 | 1.00 18.49 |
| АТОМ | | | THR | 1523 | 23.385 | -6.828 | -4.660 | 1.00 17.93 |
| АТОМ | | C | THR | 1523 | 19.806 | -8.255 | -5.065 | 1.00 15.12 |
| ATOM | | ō | THR | 1523 | 19.250 | | -6.156 | 1.00 15.12 |
| | | N | | 1524 | 19.131 | -8.323 | -3.925 | 1.00 15.13 |
| ATOM | | | ALA | | | | | |
| ATOM | | CA | ALA | 1524 | 17.675 | -8.280 | -3.889 | 1.00 12.50 |
| ATOM | | СВ | ALA | 1524 | 17.092 | -9.670 | -4.121 | 1.00 13.98 |
| ATOM | | С | ALA | 1524 | 17.296 | -7.759 | -2.508 | 1.00 13.20 |
| ATOM | | О | ALA | 1524 | 17.943 | -8.102 | -1.517 | 1.00 14.00 |
| ATOM | 10163 | N | TYR | 1525 | 16.244 | -6.946 | -2.448 | 1.00 13.12 |
| MOTA | 10164 | CA | TYR | 1525 | 15.813 | -6.346 | -1.190 | 1.00 13.36 |
| ATOM | 10165 | CB | TYR | 1525 | 16.287 | -4.896 | -1.112 | 1.00 12.75 |
| MOTA | 10166 | CG | TYR | 1525 | 17.633 | -4.646 | -1.748 | 1.00 14.96 |
| ATOM | 10167 | CD1 | TYR | 1525 | 17.717 | -4.174 | -3.056 | 1.00 16.08 |
| ATOM | | | TYR | 1525 | 18.938 | -3.904 | -3.648 | 1.00 18.05 |
| ATOM | | | TYR | 1525 | 18.820 | -4.852 | -1.040 | 1.00 15.12 |
| ATOM | | | TYR | 1525 | 20.064 | -4.582 | -1.627 | 1.00 13.12 |
| | | CZ | | 1525 | 20.107 | -4.107 | -2.928 | 1.00 16.54 |
| ATOM | | | TYR | | | | | |
| ATOM | | ОН | TYR | 1525 | 21.315 | -3.807 | -3.521 | 1.00 17.02 |
| ATOM | | С | TYR | 1525 | 14.305 | -6.357 | -0.977 | 1.00 13.91 |
| ATOM | | 0 | TYR | 1525 | 13.808 | -5.714 | -0.053 | 1.00 12.93 |
| ATOM | | N | ASP | 1526 | 13.575 | -7.055 | -1.839 | 1.00 12.13 |
| ATOM | | CA | ASP | 1526 | 12.129 | -7.127 | -1.692 | 1.00 12.96 |
| ATOM | | CB | ASP | 1526 | 11.454 | -5.901 | -2.325 | 1.00 13.73 |
| MOTA | 10178 | CG | ASP | 1526 | 11.615 | ~5.846 | -3.835 | 1.00 17.18 |
| ATOM | 10179 | OD1 | ASP | 1526 | 10.998 | -6.672 | -4.543 | 1.00 19.08 |
| ATOM | | OD2 | ASP | 1526 | 12.363 | -4.967 | -4.311 | 1.00 19.29 |
| ATOM | | С | ASP | 1526 | 11.574 | -8.412 | -2.297 | 1.00 14.23 |
| ATOM | | ō | ASP | 1526 | 12.250 | -9.088 | -3.071 | 1.00 13.08 |
| ATOM | | N | TYR | 1527 | 10.343 | -8.741 | -1.918 | 1.00 11.93 |
| ATOM | | CA | TYR | 1527 | 9.648 | -9.941 | -2.387 | 1.00 11.33 |
| | | | | | | -9.941 | | 1.00 13.10 |
| ATOM | | CB | TYR | 1527 | 8.248 | | -1.778 | |
| ATOM | | CG | TYR | 1527 | | -11.037 | -2.388 | 1.00 16.24 |
| MOTA | • | | TYR | 1527 | | -12.348 | -1.925 | 1.00 16.32 |
| MOTA | | CE1 | | 1527 | | -13.320 | -2.484 | 1.00 17.69 |
| MOTA | | CD2 | | 1527 | | -10.718 | -3.437 | 1.00 17.45 |
| MOTA | | CE2 | TYR | 1527 | | -11.688 | -4.007 | 1.00 17.34 |
| MOTA | | cz | TYR | 1527 | | -12.987 | -3.519 | 1.00 19.46 |
| MOTA | 10192 | OH | TYR | 1527 | 4.875 | -13.963 | -4.069 | 1.00 21.07 |
| | | | | | | | | |

| ATOM | 10193 | C | TYR | 1527 | 9.503 | -10.052 | -3.901 | 1.00 14.65 |
|------|-------|-----|-----|------|--------|---------|---------|------------|
| | | ō | TYR | 1527 | | -11.102 | -4.480 | 1.00 13.71 |
| MOTA | 10194 | | | | | | | |
| ATOM | 10195 | N | SER | 1528 | 9.057 | | -4.534 | 1.00 14.41 |
| MOTA | 10196 | CA | SER | 1528 | 8.825 | -9.001 | -5.965 | 1.00 12.84 |
| ATOM | 10197 | CB | SER | 1528 | 8.203 | -7.687 | -6.422 | 1.00 13.95 |
| | | | | | | | | |
| MOTA | 10198 | OG | SER | 1528 | 6.922 | | -5.821 | 1.00 16.83 |
| ATOM | 10199 | C | SER | 1528 | 10.041 | -9.324 | -6.809 | 1.00 13.31 |
| ATOM | 10200 | 0 | SER | 1528 | 9.991 | -10.229 | -7.650 | 1.00 13.87 |
| | | | | | | | | |
| MOTA | 10201 | N | PHE | 1529 | 11.139 | -8.609 | -6.610 | 1.00 13.52 |
| ATOM | 10202 | CA | PHE | 1529 | 12.315 | -8.926 | -7.410 | 1.00 14.35 |
| MOTA | 10203 | CB | PHE | 1529 | 13.359 | -7.817 | -7.299 | 1.00 12.92 |
| | | | | | | | | |
| MOTA | 10204 | CG | PHE | 1529 | 13.092 | | -8.215 | 1.00 16.39 |
| ATOM | 10205 | CD1 | PHE | 1529 | 12.474 | -5.511 | -7.747 | 1.00 15.02 |
| ATOM | 10206 | CD2 | PHE | 1529 | 13.443 | -6.743 | -9.560 | 1.00 15.32 |
| | | | | | | | | |
| MOTA | 10207 | CE1 | | 1529 | 12.207 | | -8.609 | 1.00 17.64 |
| MOTA | 10208 | CE2 | PHE | 1529 | 13.183 | -5.685 | -10.432 | 1.00 16.87 |
| MOTA | 10209 | CZ | PHE | 1529 | 12.564 | -4.529 | -9.959 | 1.00 17.73 |
| | | | | | | | | |
| MOTA | 10210 | C | PHE | 1529 | 12.909 | | -7.038 | |
| ATOM | 10211 | 0 | PHE | 1529 | 13.384 | -11.010 | -7.908 | 1.00 14.17 |
| ATOM | 10212 | N | ALA | 1530 | 12.865 | -10.628 | -5.757 | 1.00 13.05 |
| | | CA | | 1530 | | -11.925 | -5.337 | 1.00 13.28 |
| MOTA | 10213 | | ALA | | | | | |
| ATOM | 10214 | CB | ALA | 1530 | 13.261 | -12.083 | -3.819 | 1.00 11.40 |
| ATOM | 10215 | C | ALA | 1530 | 12.640 | -13.050 | -6.050 | 1.00 13.09 |
| ATOM | 10216 | 0 | ALA | 1530 | 13.242 | | -6.546 | 1.00 14.85 |
| | | | | | | | | |
| ATOM | 10217 | N | LYS | 1531 | 11.315 | -12.931 | -6.087 | 1.00 13.26 |
| ATOM | 10218 | CA | LYS | 1531 | 10.458 | -13.928 | -6.728 | 1.00 14.54 |
| ATOM | 10219 | CB | LYS | 1531 | 8 991 | -13.535 | -6.523 | 1.00 15.21 |
| | | | | | | | | |
| MOTA | 10220 | CG | LYS | 1531 | | -14.425 | -7.195 | 1.00 19.57 |
| ATOM | 10221 | CD | LYS | 1531 | 7.576 | -15.623 | -6.363 | 1.00 24.21 |
| ATOM | 10222 | CE | LYS | 1531 | 6.196 | -16.116 | -6.781 | 1.00 25.02 |
| | | | | | | | | |
| MOTA | 10223 | NZ | LYS | 1531 | | -16.393 | -8.238 | 1.00 27.58 |
| MOTA | 10224 | С | LYS | 1531 | 10.773 | -14.020 | -8.221 | 1.00 13.65 |
| ATOM | 10225 | 0 | LYS | 1531 | 10 854 | -15.114 | -8.783 | 1.00 13.38 |
| | | | | | | -12.863 | -8.853 | 1.00 15.51 |
| ATOM | 10226 | N | LEU | 1532 | | | | |
| MOTA | 10227 | CA | LEU | 1532 | 11.238 | -12.793 | -10.283 | 1.00 15.37 |
| MOTA | 10228 | CB | LEU | 1532 | 11.295 | -11.326 | -10.727 | 1.00 16.67 |
| ATOM | 10229 | CG | LEU | 1532 | | -11.051 | | 1.00 13.94 |
| | | | | | | | | |
| MOTA | 10230 | CD1 | LEU | 1532 | 11.109 | -9.614 | -12.552 | 1.00 15.17 |
| ATOM | 10231 | CD2 | LEU | 1532 | 12.937 | -11.316 | -12.617 | 1.00 18.81 |
| ATOM | 10232 | C | LEU | 1532 | | -13.507 | | 1.00 15.94 |
| | | | | | | | | |
| MOTA | 10233 | 0 | LEU | 1532 | | -14.332 | -11.522 | 1.00 18.14 |
| ATOM | 10234 | N | PHE | 1533 | 13.604 | -13.201 | -9.844 | 1.00 16.77 |
| ATOM | 10235 | CA | PHE | 1533 | 14.905 | | -10 063 | 1.00 16.92 |
| | | | | | | | | |
| MOTA | 10236 | CB | PHE | 1533 | | -13.248 | | 1.00 16.06 |
| ATOM | 10237 | CG | PHE | 1533 | 16.169 | -11.762 | -9.227 | 1.00 16.65 |
| MOTA | 10238 | CD1 | PHE | 1533 | 15.971 | -11.111 | -10 440 | 1.00 18.16 |
| | | | | | | | | |
| MOTA | 10239 | CD2 | | 1533 | 16.564 | | -8.119 | 1.00 14.45 |
| ATOM | 10240 | CE1 | PHE | 1533 | 16.157 | -9.735 | -10.554 | 1.00 18.81 |
| MOTA | 10241 | CE2 | PHE | 1533 | 16.754 | -9.632 | -8.225 | 1.00 16.25 |
| | 10242 | CZ | | 1533 | 16.549 | -8.991 | -9.443 | 1.00 18.42 |
| ATOM | | | PHE | | | | | |
| ATOM | 10243 | C | PHE | 1533 | 14.814 | -15.337 | -9.858 | 1.00 17.37 |
| ATOM | 10244 | 0 | PHE | 1533 | 15.257 | -16.112 | -10.699 | 1.00 17.81 |
| ATOM | 10245 | N | ALA | 1534 | | -15.743 | -8.732 | 1.00 17.43 |
| | | | | | | | | |
| ATOM | 10246 | CA | ALA | 1534 | | -17.159 | -8.417 | 1.00 19.85 |
| MOTA | 10247 | CB | ALA | 1534 | 13.370 | -17.333 | -7.074 | 1.00 20.47 |
| ATOM | 10248 | С | ALA | 1534 | 13.316 | -17.900 | -9.509 | 1.00 21.04 |
| | | | | | | | -9.822 | |
| MOTA | 10249 | 0 | ALA | 1534 | | -19.057 | | 1.00 19.42 |
| ATOM | 10250 | N | ASP | 1535 | 12.318 | -17.243 | -10.085 | 1.00 22.15 |
| MOTA | 10251 | CA | ASP | 1535 | 11.530 | -17.879 | -11.131 | 1.00 22.54 |
| | 10252 | СВ | | | 10.232 | | | 1.00 24.94 |
| ATOM | | | ASP | 1535 | | | | |
| ATOM | 10253 | CG | ASP | 1535 | 9.228 | -17.260 | -10.259 | 1.00 26.10 |
| ATOM | 10254 | OD1 | ASP | 1535 | 9.260 | -18.288 | -9.553 | 1.00 29.47 |
| ATOM | 10255 | | ASP | 1535 | 8.398 | | | 1.00 30.35 |
| | | | | | | | | |
| ATOM | 10256 | С | ASP | 1535 | | -18.042 | | 1.00 22.47 |
| ATOM | 10257 | 0 | ASP | 1535 | 11.874 | -18.823 | -13.296 | 1.00 22.23 |
| ATOM | 10258 | N · | GLU | 1536 | 13.386 | | | 1.00 22.56 |
| | | | | | | | | |
| ATOM | 10259 | CA | GLU | 1536 | | -17.407 | | 1.00 23.73 |
| MOTA | 10260 | CB | GLU | 1536 | 14.678 | -16.024 | -14.278 | 1.00 23.59 |
| MOTA | 10261 | CG | GLU | 1536 | 13.583 | -15.086 | -14.756 | 1.00 25.82 |
| | | | | | 12.700 | | | |
| ATOM | 10262 | CD | GLU | 1536 | | | | 1.00 26.18 |
| MOTA | 10263 | OE1 | GLU | 1536 | | -16.349 | | 1.00 25.95 |
| MOTA | 10264 | OE2 | GLU | 1536 | 11.459 | -15.575 | -15.718 | 1.00 26.71 |
| ATOM | 10265 | C | | | | -18.325 | | 1.00 24.75 |
| | | | GLU | 1536 | | | | |
| MOTA | 10266 | 0 | GLU | 1536 | 15.973 | -18.784 | | 1.00 26.28 |
| ATOM | 10267 | N | GLY | 1537 | 15.797 | -18.583 | -12.433 | 1.00 25.87 |
| ATOM | 10268 | CA | GLY | 1537 | | -19.447 | | 1.00 25.64 |
| | | | | | | | | |
| MOTA | 10269 | С | GLY | 1537 | 18.037 | -18.855 | -11.356 | 1.00 24.92 |

| ATOM | 10270 | 0 | GLY | 1537 | 18.903 | -19.588 | -10.893 | 1.00 26.48 |
|--------|-------|-----|------|------|--------|---------|---------|------------|
| ATOM | 10271 | N | LEU | 1538 | 18.014 | -17.540 | -11.148 | 1.00 23.82 |
| ATOM | 10272 | CA | LEU | 1538 | 19.010 | -16.872 | | 1.00 24.22 |
| ATOM | 10272 | CB | LEU | 1538 | 18.938 | -15.356 | | 1.00 24.47 |
| ATOM | 10274 | CG | LEU | 1538 | | -14.653 | | 1.00 26.59 |
| | | | | | | -13.170 | | 1.00 23.00 |
| ATOM | 10275 | | LEU | 1538 | | | | |
| MOTA | 10276 | | LEU | 1538 | 21.403 | -14.879 | | 1.00 25.88 |
| MOTA | 10277 | С | LEU | 1538 | | -17.223 | -8.862 | 1.00 23.54 |
| MOTA | 10278 | 0 | LEU | 1538 | | -16.580 | -8.246 | 1.00 22.67 |
| ATOM | 10279 | N | ASN | 1539 | 19.372 | -18.235 | -8.338 | 1.00 23.14 |
| ATOM | 10280 | CA | ASN | 1539 | 19.146 | -18.740 | -6.985 | 1.00 23.02 |
| ATOM | 10281 | CB | ASN | 1539 | 19.144 | -20.276 | -6.991 | 1.00 25.31 |
| MOTA | 10282 | CG | ASN | 1539 | 18.057 | -20.857 | -7.877 | 1.00 29.87 |
| ATOM | 10283 | | ASN | 1539 | 16.946 | -20.333 | -7.935 | 1.00 31.66 |
| ATOM | 10284 | ND2 | | 1539 | | -21.956 | -8.560 | 1.00 32.41 |
| ATOM | 10285 | C | ASN | 1539 | | -18.266 | -5.905 | 1.00 21.17 |
| ATOM | 10286 | ō | ASN | 1539 | | -18.785 | -4.787 | 1.00 22.27 |
| ATOM | 10287 | N | VAL | 1540 | | -17.303 | -6.229 | 1.00 18.20 |
| | | CA | | 1540 | 21.922 | -16.778 | -5.255 | 1.00 17.11 |
| ATOM | 10288 | | VAL | | | -17.043 | -5.672 | 1.00 17.11 |
| ATOM | 10289 | CB | VAL | 1540 | 23.383 | | | |
| ATOM | 10290 | | VAL | 1540 | 24.322 | -16.576 | -4.558 | 1.00 19.33 |
| ATOM | 10291 | CG2 | | 1540 | 23.583 | -18.517 | -5.941 | 1.00 17.44 |
| MOTA | 10292 | С | VAL | 1540 | | -15.284 | -5.161 | 1.00 15.86 |
| MOTA | 10293 | 0 | VAL | 1540 | | -14.537 | -6.113 | 1.00 14.51 |
| MOTA | 10294 | N | MET | 1541 | | -14.845 | -4.008 | 1.00 14.44 |
| ATOM | 10295 | CA | MET | 1541 | 20.921 | -13.437 | -3.815 | 1.00 14.69 |
| ATOM | 10296 | CB | MET | 1541 | 19.408 | -13.226 | -3.696 | 1.00 16.00 |
| ATOM | 10297 | CG | MET | 1541 | 18.661 | -13.438 | -4.990 | 1.00 17.44 |
| ATOM | 10298 | SD | MET | 1541 | 16.908 | -13.405 | -4.789 | 1.00 18.84 |
| ATOM | 10299 | CE | MET | 1541 | | -15.008 | -5.443 | 1.00 17.64 |
| ATOM | 10300 | C | MET | 1541 | | -12.869 | -2.586 | 1.00 14.81 |
| ATOM | 10300 | 0 | MET | 1541 | 21.776 | -13.564 | -1.587 | 1.00 15.31 |
| | | | | 1542 | 21.776 | -11.585 | -2.656 | 1.00 13.31 |
| ATOM | 10302 | N | LEU | | | | -1.537 | 1.00 13.41 |
| ATOM | 10303 | CA | LEU | 1542 | 22.518 | -10.920 | | |
| ATOM | 10304 | CB | LEU | 1542 | | -10.527 | -1.929 | 1.00 16.33 |
| ATOM | 10305 | CG | LEU | 1542 | 24.874 | -9.753 | -0.982 | 1.00 22.57 |
| MOTA | 10306 | | LEU | 1542 | 24.655 | -8.278 | -1.204 | 1.00 25.11 |
| MOTA | 10307 | CD2 | LEU | 1542 | 24.678 | -10.149 | 0.485 | 1.00 19.55 |
| MOTA | 10308 | C | LEU | 1542 | 21.726 | -9.706 | -1.077 | 1.00 11.50 |
| MOTA | 10309 | 0 | LEU | 1542 | 21.406 | -8.814 | -1.862 | 1.00 11.99 |
| MOTA | 10310 | N | VAL | 1543 | 21.394 | -9.701 | 0.210 | 1.00 12.88 |
| MOTA | 10311 | CA | VAL | 1543 | 20.685 | -8.590 | 0.805 | 1.00 12.95 |
| MOTA | 10312 | CB | VAL | 1543 | 19.750 | -9.067 | 1.918 | 1.00 14.28 |
| ATOM | 10313 | | VAL | 1543 | 19.016 | -7.885 | 2.529 | 1.00 15.11 |
| ATOM | 10314 | CG2 | VAL | 1543 | 18.759 | -10.079 | 1.344 | 1.00 13.81 |
| ATOM | 10315 | C | VAL | 1543 | 21.838 | -7.785 | 1.377 | 1.00 14.63 |
| ATOM | 10316 | o | VAL | 1543 | 22.264 | -7.998 | 2.516 | 1.00 14.81 |
| | | N | | 1544 | 22.362 | -6.883 | 0.557 | 1.00 14.42 |
| MOTA | 10317 | | GLY | | | | 0.966 | 1.00 14.42 |
| MOTA | 10318 | CA | GLY | 1544 | 23.503 | -6.088 | | |
| MOTA | 10319 | C | GLY | 1544 | 23.197 | -4.703 | 1.471 | 1.00 16.06 |
| MOTA | 10320 | 0 | GLY | 1544 | 22.122 | -4.155 | 1.207 | 1.00 17.57 |
| MOTA | 10321 | N | ASP | 1545 | 24.153 | -4.126 | | 1.00 16.67 |
| ATOM | 10322 | CA | ASP | 1545 | 23.945 | -2.796 | 2.730 | 1.00 16.34 |
| MOTA | 10323 | CB | ASP | 1545 | 24.990 | -2.444 | 3.808 | 1.00 18.01 |
| MOTA | 10324 | CG | ASP | 1545 | 26.422 | -2.547 | 3.324 | 1.00 17.58 |
| MOTA | 10325 | OD1 | ASP | 1545 | 26.656 | -2.778 | 2.126 | 1.00 18.33 |
| MOTA | 10326 | OD2 | ASP | 1545 | 27.321 | -2.384 | 4.171 | 1.00 20.23 |
| ATOM | 10327 | С | ASP | 1545 | 23.910 | -1.765 | 1.613 | 1.00 15.12 |
| ATOM | 10328 | ō | ASP | 1545 | 23.718 | -0.578 | 1.860 | 1.00 17.15 |
| ATOM | 10329 | N | SER | 1546 | 24.066 | -2.223 | 0.373 | 1.00 15.22 |
| ATOM | 10330 | CA | SER | 1546 | 23.966 | -1.307 | -0.752 | 1.00 13.69 |
| ATOM | | CB | SER | 1546 | 24.223 | -2.036 | -2.077 | 1.00 16.92 |
| | 10331 | | | | 23.495 | -3.253 | -2.157 | 1.00 16.32 |
| ATOM | 10332 | OG | SER | 1546 | | | | i |
| ATOM | 10333 | C | SER | 1546 | 22.554 | -0.721 | -0.725 | 1.00 15.02 |
| ATOM | 10334 | 0 | SER | 1546 | 22.302 | 0.346 | -1.289 | 1.00 16.38 |
| ATOM | 10335 | N | LEU | 1547 | 21.627 | -1.411 | -0.057 | 1.00 13.61 |
| MOTA | 10336 | CA | LEU | 1547 | 20.255 | -0.904 | 0.033 | 1.00 13.00 |
| ATOM | 10337 | CB | LEU | 1547 | 19.359 | -1.891 | 0.804 | 1.00 14.09 |
| MOTA | 10338 | CG | LEU | 1547 | 19.730 | -2.207 | 2.259 | 1.00 11.97 |
| ATOM | 10339 | | LEU | 1547 | 19.088 | -1.193 | 3.174 | 1.00 17.68 |
| ATOM | 10340 | CD2 | LEU | 1547 | 19.261 | -3.621 | 2.631 | 1.00 16.59 |
| MOTA | 10341 | С | LEU | 1547 | 20.246 | 0.471 | 0.711 | 1.00 13.72 |
| ATOM | 10342 | 0 | LEU | 1547 | 19.303 | 1.249 | 0.556 | 1.00 12.82 |
| MOTA | 10343 | N | GLY | 1548 | 21.302 | 0.768 | 1.462 | 1.00 14.37 |
| MOTA | 10344 | CA | GLY | 1548 | 21.386 | 2.059 | 2.128 | 1.00 13.78 |
| ATOM | 10345 | C | GLY | 1548 | 21.310 | 3.187 | 1.120 | 1.00 15.41 |
| MOTA | 10345 | 0 | GLY | 1548 | 20.786 | 4.267 | 1.403 | 1.00 15.37 |
| 211 OF | 70740 | J | -LII | 7J40 | 20.700 | 1.207 | 1.103 | , |
| | | | | | | | | |

| АТОМ | 10347 | N | MET | 1549 | 21.805 | 2.914 | -0.083 | 1.00 16.39 |
|--------------|----------------|----------|------------|--------------|------------------|-----------------|------------------|--------------------------|
| MOTA | 10348 | CA | MET | 1549 | 21.825 | 3.900 | -1.151 | 1.00 16.76 |
| MOTA | 10349 | CB | MET | 1549 | 23.198 | 3.852 | -1.842 | 1.00 18.82 |
| MOTA | 10350 | CG | MET | 1549 | 24.346 | 4.147 | -0.882 | 1.00 20.11 |
| MOTA | 10351 | SD | MET | 1549 | 26.012 | 3.963 | -1.563 | 1.00 26.68 |
| MOTA | 10352 | CE | MET | 1549 | 26.138 | 5.439 | -2.542 | 1.00 27.73 |
| MOTA | 10353 10354 | C 0 | MET MET | 1549 1549 | 20.696 19.935 | 3.703 4.627 | -2.165 -2.443 | 1.00 17.66 1.00 19.20 |
| MOTA MOTA | 10354 | N | THR | 1550 | 20.567 | 2.495 | -2.700 | 1.00 17.07 |
| ATOM | 10356 | CA | THR | 1550 | 19.529 | 2.234 | -3.693 | 1.00 17.56 |
| ATOM | 10357 | СВ | THR | 1550 | 19.809 | 0.931 | -4.439 | 1.00 21.36 |
| MOTA | 10358 | OG1 | THR | 1550 | 18.737 | 0.665 | -5.349 | 1.00 29.04 |
| MOTA | 10359 | CG2 | THR | 1550 | 19.953 | -0.219 | -3.472 | 1.00 19.69 |
| MOTA | 10360 | C | THR | 1550 | 18.103 | 2.191 | -3.143 | 1.00 17.30 |
| MOTA | 10361 | 0 | THR | 1550 | 17.144 | 2.507 | -3.853 | 1.00 19.51 |
| MOTA | 10362 | N | VAL VAL | 1551 1551 | 17.949 16.616 | 1.800 1.741 | -1.884 -1.297 | 1.00 16.88 1.00 15.66 |
| MOTA MOTA | 10363 10364 | CA CB | VAL | 1551 | 16.412 | 0.423 | -0.504 | 1.00 15.00 |
| ATOM | 10365 | CG1 | | 1551 | 15.077 | 0.454 | 0.240 | 1.00 15.49 |
| ATOM | 10366 | | VAL | 1551 | 16.436 | -0.760 | -1.452 | 1.00 17.32 |
| MOTA | 10367 | С | VAL | 1551 | 16.344 | 2.929 | -0.377 | 1.00 14.94 |
| MOTA | 10368 | 0 | VAL | 1551 | 15.351 | 3.635 | -0.540 | 1.00 13.06 |
| MOTA | 10369 | N | GLN | 1552 | 17.231 | 3.155 | 0.584 | 1.00 13.60 |
| MOTA | 10370 | CA | GLN | 1552 | 17.041 | 4.242 | 1.536 | 1.00 13.62 |
| MOTA | 10371 | CB | GLN | 1552 | 17.857 | 3.963 2.569 | 2.798 3.329 | 1.00 14.36 1.00 15.64 |
| ATOM ATOM | 10372 10373 | CG CD | GLN GLN | 1552 1552 | 17.589 18.298 | 2.290 | 4.628 | 1.00 13.04 |
| ATOM | 10373 | OE1 | | 1552 | 19.342 | 2.875 | 4.914 | 1.00 17.01 |
| ATOM | 10375 | | GLN | 1552 | 17.744 | 1.372 | 5.418 | 1.00 12.68 |
| ATOM | 10376 | С | GLN | 1552 | 17.396 | 5.610 | 0.968 | 1.00 12.37 |
| ATOM | 10377 | 0 | GLN | 1552 | 16.852 | 6.625 | 1.403 | 1.00 13.34 |
| MOTA | 10378 | N | GLY | 1553 | 18.312 | 5.643 | 0.007 | 1.00 13.54 |
| MOTA | 10379 | CA | GLY | 1553 | 18.679 | 6.914 | -0.585 | 1.00 12.70 |
| MOTA | 10380 | C | GLY | 1553 | 19.761 | 7.687 | 0.140 | 1.00 16.01 1.00 14.75 |
| MOTA MOTA | 10381 10382 | O N | GLY HIS | 1553 1554 | 19.859 20.563 | 8.905 6.999 | -0.013 0.948 | 1.00 14.75 1.00 16.13 |
| ATOM | 10382 | CA | HIS | 1554 | 21.659 | 7.665 | 1.655 | 1.00 19.25 |
| ATOM | 10384 | СВ | HIS | 1554 | 22.058 | 6.870 | 2.901 | 1.00 18.68 |
| ATOM | 10385 | CG | HIS | 1554 | 21.002 | 6.837 | 3.962 | 1.00 18.56 |
| MOTA | 10386 | | HIS | 1554 | 20.261 | 5.814 | 4.452 | 1.00 18.97 |
| MOTA | 10387 | ND1 | | 1554 | 20.599 | 7.964 | 4.646 | 1.00 19.57 |
| ATOM | 10388 | CE1 | | 1554 | 19.654 19.429 | 7.637 6.338 | 5.509 5.412 | 1.00 21.71 1.00 16.82 |
| ATOM ATOM | 10389 10390 | NE2 | HIS HIS | 1554 1554 | 22.845 | 7.761 | 0.692 | 1.00 10.82 |
| ATOM | 10391 | 0 | HIS | 1554 | 22.867 | 7.081 | -0.332 | 1.00 20.01 |
| MOTA | 10392 | N | ASP | 1555 | 23.824 | 8.604 | 1.023 | 1.00 23.52 |
| ATOM. | 10393 | CA | ASP | 1555 | 25.007 | 8.786 | 0.182 | 1.00 25.86 |
| ATOM | 10394 | CB | ASP | 1555 | 25.650 | 10.153 | 0.451 | 1.00 31.31 |
| MOTA | 10395 | CG | ASP | 1555 | 25.964 | 10.375 | 1.919 | 1.00 34.15 |
| MOTA | 10396 | OD1 | | 1555 | 26.709 25.461 | 9.570 | 2.509 2.489 | 1.00 37.32 1.00 40.85 |
| MOTA MOTA | 10397 10398 | OD2 C | ASP | 1555 1555 | 26.055 | 11.366 7.695 | 0.374 | 1.00 40.83 |
| MOTA | 10399 | 0 | ASP | 1555 | 27.045 | 7.637 | -0.356 | 1.00 27.92 |
| ATOM | 10400 | N | SER | 1556 | 25.841 | 6.832 | 1.359 | 1.00 21.86 |
| MOTA | 10401 | CA | SER | 1556 | 26.769 | 5.742 | 1.627 | 1.00 19.58 |
| MOTA | 10402 | CB | SER | 1556 | 27.890 | 6.195 | 2.569 | 1.00 18.25 |
| MOTA | 10403 | OG | SER | 1556 | 27.408 | 6.452 | 3.880 | 1.00 19.02 |
| ATOM | 10404 | С | SER SER | 1556 1556 | 25.987 24.791 | 4.608 4.739 | 2.264 2.491 | 1.00 18.25 1.00 16.30 |
| ATOM ATOM | 10405 10406 | O N | THR | 1557 | 26.665 | 3.505 | 2.560 | 1.00 16.50 |
| ATOM | 10407 | CA | THR | 1557 | 26.011 | 2.353 | 3.156 | 1.00 16.89 |
| MOTA | 10408 | CB | THR | 1557 | 26.639 | 1.033 | 2.664 | 1.00 17.09 |
| MOTA | 10409 | OG1 | THR | 1557 | 27.965 | 0.921 | 3.192 | 1.00 17.06 |
| MOTA | 10410 | CG2 | THR | 1557 | 26.698 | 0.996 | 1.134 | 1.00 17.62 |
| MOTA | 10411 | C | THR | 1557 | 26.079 | 2.350 | 4.682 | 1.00 16.25 1.00 16.54 |
| MOTA MOTA | 10412 | O N | THR | 1557 1558 | 25.424 26.858 | 1.530 3.257 | 5.315 5.274 | 1.00 16.54 |
| ATOM | 10413 10414 | CA | LEU LEU | 1558 | 27.018 | 3.301 | 6.738 | 1.00 15.88 |
| ATOM | 10415 | CB | LEU | 1558 | 27.954 | 4.450 | 7.141 | 1.00 17.19 |
| ATOM | 10416 | CG | LEU | 1558 | 29.465 | 4.181 | 7.061 | 1.00 17.43 |
| MOTA | 10417 | CD1 | | 1558 | 29.864 | 3.894 | 5.620 | 1.00 17.48 |
| MOTA | 10418 | | LEU | 1558 | 30.223 | 5.395 | 7.599 | 1.00 18.51 |
| ATOM | 10419 | C | LEU | 1558 | 25.747 | 3.376 | 7.596 | 1.00 15.47 |
| ATOM | 10420 | O N | LEU | 1558 1559 | 25.676 24.736 | 2.770 4.134 | 8.666 7.156 | 1.00 14.85 1.00 16.50 |
| ATOM ATOM | 10421 10422 | N CD | PRO PRO | 1559 | 24.738 | 5.128 | 6.072 | 1.00 15.31 |
| ATOM | 10423 | CA | PRO | 1559 | 23.507 | 4.227 | 7.951 | 1.00 15.63 |

| ATOM | 10424 | CB | PRO | 1559 | 22.736 | 5.358 | 7.271 | 1.00 18.98 |
|------|-------|-----|-----|--------------|--------|---------|---------|------------|
| ATOM | 10425 | CG | PRO | 1559 | 23.279 | 5.362 | 5.865 | 1.00 21.76 |
| MOTA | 10426 | С | PRO | 1559 | 22.685 | 2.940 | 8.055 | 1.00 15.29 |
| ATOM | 10427 | 0 | PRO | 1559 | 21.786 | 2.840 | 8.894 | 1.00 16.41 |
| ATOM | 10428 | N | VAL | 1560 | 22.988 | 1.951 | 7.223 | 1.00 14.37 |
| ATOM | 10429 | CA | VAL | 1560 | 22.236 | 0.703 | 7.263 | 1.00 13.86 |
| | | CB | | 1560 | 22.636 | | | |
| MOTA | 10430 | | VAL | | | -0.220 | 6.088 | |
| MOTA | 10431 | | VAL | 1560 | 21.928 | -1.553 | 6.199 | 1.00 15.90 |
| MOTA | 10432 | | VAL | 1560 | 22.293 | 0.446 | 4.773 | 1.00 12.67 |
| ATOM | 10433 | С | VAL | 1560 | 22.500 | -0.025 | 8.579 | 1.00 13.66 |
| ATOM | 10434 | 0 | VAL | 1560 | 23.653 | -0.180 | 8.993 | 1.00 12.04 |
| ATOM | 10435 | N | THR | 1561 | 21.448 | -0.467 | 9.254 | 1.00 14.89 |
| ATOM | 10436 | CA | THR | 1561 | 21.676 | -1.191 | 10.500 | 1.00 18.92 |
| ATOM | 10437 | CB | THR | 1561 | 21.076 | -0.416 | 11.713 | 1.00 25.70 |
| ATOM | 10438 | OG1 | THR | 1561 | 22.006 | 0.601 | 12.128 | 1.00 30.54 |
| ATOM | 10439 | CG2 | THR | 1561 | 20.806 | -1.340 | 12.899 | 1.00 27.97 |
| MOTA | 10440 | С | THR | 1561 | 21.179 | -2.632 | 10.388 | 1.00 17.00 |
| ATOM | 10441 | ō | THR | 1561 | 20.535 | -2.998 | 9.405 | 1.00 13.03 |
| ATOM | 10442 | N | VAL | 1562 | 21.516 | -3.458 | 11.375 | 1.00 14.93 |
| ATOM | 10443 | CA | VAL | 1562 | 21.134 | -4.868 | 11.378 | 1.00 13.72 |
| ATOM | 10443 | CB | VAL | 1562 | 21.617 | -5.554 | 12.691 | 1.00 13.72 |
| | | | | | | -7.006 | 12.747 | 1.00 14.34 |
| ATOM | 10445 | | VAL | 1562 | 21.157 | | | |
| ATOM | 10446 | CG2 | | 1562 | 23.136 | -5.481 | 12.760 | 1.00 15.87 |
| ATOM | 10447 | C | VAL | 1562 | 19.633 | -5.044 | 11.218 | 1.00 13.79 |
| ATOM | 10448 | 0 | VAL | 1562 | 19.184 | -5.919 | 10.477 | 1.00 11.90 |
| MOTA | 10449 | N | ALA | 1563 | 18.862 | -4.205 | 11.906 | 1.00 12.57 |
| MOTA | 10450 | CA | ALA | 1563 | 17.410 | -4.266 | 11.818 | 1.00 13.52 |
| ATOM | 10451 | CB | ALA | 1563 | 16.793 | -3.175 | 12.665 | 1.00 15.49 |
| ATOM | 10452 | С | ALA | 1563 | 16.967 | -4.106 | 10.367 | 1.00 13.22 |
| MOTA | 10453 | 0 | ALA | 1563 | 16.055 | -4.796 | 9.905 | 1.00 11.97 |
| ATOM | 10454 | N | ASP | 1564 | 17.603 | -3.185 | 9.649 | 1.00 13.76 |
| ATOM | 10455 | CA | ASP | 1564 | 17.258 | -2.973 | 8.243 | 1.00 14.61 |
| ATOM | 10456 | СВ | ASP | 1564 | 18.111 | -1.873 | 7.601 | 1.00 12.63 |
| ATOM | 10457 | CG | ASP | 1564 | 17.836 | -0.491 | 8.172 | 1.00 15.27 |
| ATOM | 10457 | | ASP | 1564 | 16.732 | -0.262 | 8.711 | 1.00 13.27 |
| | | | | | | | | 1.00 12.78 |
| ATOM | 10459 | | ASP | 1564 | 18.735 | 0.359 | 8.042 | |
| ATOM | 10460 | C | ASP | 1564 | 17.501 | -4.243 | 7.448 | 1.00 13.99 |
| ATOM | 10461 | 0 | ASP | 1564 | 16.647 | -4.696 | 6.685 | 1.00 12.31 |
| ATOM | 10462 | N | ILE | 1565 | 18.696 | -4.802 | 7.602 | 1.00 12.52 |
| MOTA | 10463 | CA | ILE | 1565 | 19.042 | -6.019 | 6.878 | 1.00 11.04 |
| MOTA | 10464 | CB | ILE | 1565 | 20.450 | -6.514 | 7.251 | 1.00 12.44 |
| ATOM | 10465 | CG2 | ILE | 1565 | 20.699 | 7.867 | 6.594 | 1.00 12.14 |
| ATOM | 10466 | CG1 | ILE | 1565 | 21.501 | -5.478 | 6.817 | 1.00 9.14 |
| MOTA | 10467 | CD1 | ILE | 1565 | 21.658 | -5.322 | 5.303 | 1.00 13.72 |
| MOTA | 10468 | С | ILE | 1565 | 18.034 | -7.132 | 7.160 | 1.00 11.12 |
| ATOM | 10469 | 0 | ILE | 1565 | 17.606 | -7.822 | 6.247 | 1.00 10.33 |
| ATOM | 10470 | N | ALA | 1566 | 17.651 | -7.309 | 8.422 | 1.00 9.51 |
| ATOM | 10471 | CA | ALA | 1566 | 16.699 | -8.364 | 8.743 | 1.00 10.56 |
| ATOM | 10472 | СВ | ALA | 1566 | 16.495 | -8.460 | 10.241 | 1.00 10.34 |
| ATOM | 10473 | C | ALA | 1566 | 15.365 | -8.141 | 8.050 | 1.00 8.48 |
| ATOM | 10474 | ō | ALA | 1566 | 14.744 | -9.084 | 7.553 | 1.00 10.65 |
| | | | TYR | | | | 8.028 | 1.00 10.03 |
| MOTA | 10475 | N | | 1567 1567 | 14.919 | -6.894 | | 1.00 10.49 |
| MOTA | 10476 | CA | TYR | | 13.644 | -6.538 | 7.394 | |
| MOTA | 10477 | CB | TYR | 1567 | 13.426 | -5.023 | 7.478 | 1.00 11.37 |
| MOTA | 10478 | CG | TYR | 1567 | 12.216 | -4.515 | 6.708 | 1.00 13.66 |
| MOTA | 10479 | CD1 | TYR | 1567 | 10.925 | -4.761 | 7.163 | 1.00 12.46 |
| MOTA | 10480 | CE1 | TYR | 1567 | 9.816 | -4.222 | 6.513 | 1.00 14.53 |
| MOTA | 10481 | CD2 | TYR | 1567 | 12.373 | -3.724 | - 5.568 | 1.00 15.00 |
| ATOM | 10482 | CE2 | TYR | 1567 | 11.277 | -3.180 | 4.909 | 1.00 14.51 |
| MOTA | 10483 | CZ | TYR | 1567 | 10.002 | -3.429 | 5.391 | 1.00 14.84 |
| ATOM | 10484 | OH | TYR | 1567 | 8.917 | -2.852 | 4.784 | 1.00 13.91 |
| MOTA | 10485 | С | TYR | 1567 | 13.639 | -6.960 | 5.933 | 1.00 10.89 |
| ATOM | 10486 | 0 | TYR | 1567 | 12.708 | -7.617 | 5.460 | 1.00 10.65 |
| ATOM | 10487 | N | HIS | 1568 | 14.682 | -6.558 | 5.217 | 1.00 10.43 |
| ATOM | 10488 | CA | HIS | 1568 | 14.775 | -6.881 | 3.801 | 1.00 10.21 |
| MOTA | 10489 | CB | HIS | 1568 | 15.842 | -5.998 | 3.140 | 1.00 11.31 |
| ATOM | 10490 | CG | HIS | 1568 | 15.411 | -4.565 | 2.971 | 1.00 11.56 |
| ATOM | 10491 | | HIS | 1568 | 15.646 | -3.467 | 3.731 | 1.00 11.50 |
| | 10491 | | HIS | | | -4.149 | 1.953 | 1.00 11.31 |
| MOTA | | | | 1568 | 14.579 | | | |
| MOTA | 10493 | | HIS | 1568 | 14.319 | -2.861 | 2.091 | 1.00 13.74 |
| MOTA | 10494 | | HIS | 1568 | 14.954 | -2.422 | 3.163 | 1.00 12.66 |
| ATOM | 10495 | C | HIS | 1568 | 15.044 | -8.370 | 3.594 | 1.00 11.46 |
| MOTA | 10496 | 0 | HIS | 1568 | 14.540 | -8.977 | 2.643 | 1.00 10.22 |
| MOTA | 10497 | N | THR | 1569 | 15.819 | -8.970 | 4.492 | 1.00 10.71 |
| MOTA | 10498 | CA | THR | 1569 | 16.104 | -10.397 | 4.390 | 1.00 10.69 |
| MOTA | 10499 | CB | THR | 1569 | 17.054 | -10.853 | 5.521 | 1.00 12.47 |
| MOTA | 10500 | OG1 | THR | 1569 | 18.347 | -10.273 | 5.306 | 1.00 10.54 |

| ATOM | 10501 | CG2 | THR | 1569 | 17.169 -12.392 | 5.559 | 1.00 11.72 |
|------|-------|-----|-------|------|----------------|--------|------------|
| ATOM | 10502 | С | THR | 1569 | 14.822 -11.236 | 4.436 | 1.00 12.77 |
| ATOM | 10503 | 0 | THR | 1569 | 14.657 -12.170 | 3.646 | 1.00 11.27 |
| ATOM | 10504 | N | ALA | 1570 | 13.915 -10.915 | 5.359 | 1.00 11.72 |
| ATOM | 10505 | CA | ALA | 1570 | 12.666 -11.671 | 5.471 | 1.00 13.45 |
| ATOM | 10506 | CB | ALA | 1570 | 11.861 -11.200 | 6.689 | 1.00 12.98 |
| | | C | ALA | 1570 | 11.819 -11.544 | 4.211 | 1.00 12.73 |
| ATOM | 10507 | | | | | | |
| ATOM | 10508 | 0 | ALA | 1570 | 11.182 -12.506 | 3.784 | 1.00 13.55 |
| MOTA | 10509 | N | ALA | 1571 | 11.804 -10.348 | 3.628 | 1.00 12.25 |
| MOTA | 10510 | CA | ALA | 1571 | 11.028 -10.110 | 2.422 | 1.00 10.68 |
| ATOM | 10511 | CB | ALA | 1571 | 11.014 -8.619 | 2.086 | 1.00 10.51 |
| ATOM | 10512 | С | ALA | 1571 | 11.615 -10.907 | 1.262 | 1.00 11.99 |
| ATOM | 10513 | 0 | ALA | 1571 | 10.881 -11.499 | 0.477 | 1.00 11.47 |
| ATOM | 10514 | N | VAL | 1572 | 12.939 -10.923 | 1.144 | 1.00 13.05 |
| ATOM | 10515 | CA | VAL | 1572 | 13.553 -11.687 | 0.064 | 1.00 13.95 |
| ATOM | 10516 | CB | VAL | 1572 | 15.075 -11.473 | 0.004 | 1.00 13.81 |
| ATOM | 10517 | | VAL | 1572 | 15.701 -12.485 | -0.954 | 1.00 14.45 |
| ATOM | 10518 | CG2 | | 1572 | 15.379 -10.050 | -0.458 | 1.00 14.01 |
| MOTA | 10519 | C | VAL | 1572 | 13.271 -13.178 | 0.239 | 1.00 14.25 |
| | | | | | | -0.727 | 1.00 14.23 |
| MOTA | 10520 | 0 | VAL | 1572 | 12.956 -13.888 | | |
| MOTA | 10521 | N | ARG | 1573 | 13.388 -13.659 | 1.471 | 1.00 13.28 |
| MOTA | 10522 | CA | ARG | 1573 | 13.137 -15.066 | 1.733 | 1.00 12.96 |
| MOTA | 10523 | CB | ARG | 1573 | 13.418 -15.409 | 3.208 | 1.00 12.40 |
| MOTA | 10524 | CG | ARG | 1573 | 13.134 -16.875 | 3.564 | 1.00 14.12 |
| MOTA | 10525 | CD | ARG | 1573 | 13.891 -17.820 | 2.636 | 1.00 11.99 |
| ATOM | 10526 | NE | ARG | 1573 | 15.299 -17.944 | 3.009 | 1.00 15.31 |
| ATOM | 10527 | CZ | ARG | 1573 | 16.238 -18.497 | 2.248 | 1.00 17.73 |
| ATOM | 10528 | NH1 | ARG | 1573 | 15.931 -18.981 | 1.048 | 1.00 18.85 |
| MOTA | 10529 | NH2 | | 1573 | 17.486 -18.589 | 2.696 | 1.00 15.43 |
| ATOM | 10530 | C | ARG | 1573 | 11.701 -15.460 | 1.358 | 1.00 12.91 |
| ATOM | 10531 | o | ARG | 1573 | 11.467 -16.569 | 0.882 | 1.00 14.66 |
| | 10531 | | | 1574 | 10.740 -14.561 | 1.559 | 1.00 15.46 |
| ATOM | | N | ARG | | 9.356 -14.883 | | |
| ATOM | 10533 | CA | ARG | 1574 | | 1.214 | 1.00 13.92 |
| MOTA | 10534 | CB | ARG | 1574 | 8.392 -13.802 | 1.707 | 1.00 14.87 |
| MOTA | 10535 | CG | ARG | 1574 | 8.358 -13.622 | 3.212 | 1.00 17.41 |
| MOTA | 10536 | CD | ARG . | | 7.182 -12.767 | 3.655 | 1.00 17.23 |
| ATOM | 10537 | NE | ARG | 1574 | 7.241 -12.534 | 5.096 | 1.00 19.59 |
| MOTA | 10538 | CZ | ARG | 1574 | 7.851 -11.505 | 5.673 | 1.00 20.15 |
| ATOM | 10539 | NH1 | ARG | 1574 | 8.459 -10.577 | 4.939 | 1.00 17.97 |
| ATOM | 10540 | NH2 | ARG | 1574 | 7.882 -11.421 | 6.995 | 1.00 23.22 |
| ATOM | 10541 | С | ARG | 1574 | 9.210 -15.013 | -0.294 | 1.00 13.49 |
| ATOM | 10542 | 0 | ARG | 1574 | 8.380 -15.777 | -0.786 | 1.00 14.10 |
| MOTA | 10543 | N | GLY | 1575 | 10.017 -14.256 | -1.024 | 1.00 12.47 |
| ATOM | 10544 | CA | GLY | 1575 | 9.949 -14.297 | -2.474 | 1.00 15.24 |
| ATOM | 10545 | C | GLY | 1575 | 10.693 -15.461 | -3.096 | 1.00 16.10 |
| | | | | | | | |
| ATOM | 10546 | 0 | GLY | 1575 | 10.307 -15.961 | -4.150 | 1.00 17.71 |
| ATOM | 10547 | N | ALA | 1576 | 11.761 -15.894 | -2.441 | 1.00 15.51 |
| MOTA | 10548 | CA | ALA | 1576 | 12.577 -16.990 | -2.950 | 1.00 16.76 |
| ATOM | 10549 | CB | ALA | 1576 | 13.834 -16.430 | -3.584 | 1.00 18.02 |
| ATOM | 10550 | С | ALA | 1576 | 12.935 -17.923 | -1.800 | 1.00 16.86 |
| MOTA | 10551 | 0 | ALA | 1576 | 14.065 -17.923 | -1.318 | 1.00 17.30 |
| MOTA | 10552 | N | PRO | 1577 | 11.977 -18.756 | -1.368 | 1.00 18.36 |
| MOTA | 10553 | CD | PRO | 1577 | 10.647 -18.935 | -1.980 | 1.00 17.74 |
| ATOM | 10554 | CA | PRO | 1577 | 12.176 -19.696 | -0.262 | 1.00 19.18 |
| MOTA | 10555 | CB | PRO | 1577 | 10.783 -20.287 | -0.063 | 1.00 19.74 |
| ATOM | 10556 | CG | PRO | 1577 | 10.218 -20.291 | -1.442 | 1.00 22.52 |
| ATOM | 10557 | C | PRO | 1577 | 13.255 -20.767 | -0.421 | 1.00 21.10 |
| ATOM | 10558 | ō | PRO | 1577 | 13.664 -21.380 | 0.566 | 1.00 21.21 |
| ATOM | 10559 | N | ASN | 1578 | 13.725 -20.987 | -1.647 | 1.00 19.12 |
| ATOM | 10560 | CA | | 1578 | 14.741 -22.008 | -1.879 | 1.00 19.33 |
| | | | ASN | | | -2.898 | |
| ATOM | 10561 | CB | ASN | 1578 | 14.237 -23.029 | | |
| ATOM | 10562 | CG | ASN | 1578 | 12.980 -23.737 | -2.435 | 1.00 26.55 |
| MOTA | 10563 | | ASN | 1578 | 12.942 -24.304 | -1.344 | 1.00 30.38 |
| MOTA | 10564 | | ASN | 1578 | 11.942 -23.707 | -3.266 | 1.00 30.04 |
| MOTA | 10565 | С | ASN | 1578 | 16.077 -21.465 | -2.347 | 1.00 18.42 |
| MOTA | 10566 | 0 | ASN | 1578 | 16.972 -22.230 | -2.711 | 1.00 17.87 |
| MOTA | 10567 | N | CYS | 1579 | 16.230 -20.148 | -2.333 | 1.00 16.75 |
| MOTA | 10568 | CA | CYS | 1579 | 17.486 -19.565 | -2.794 | 1.00 16.63 |
| MOTA | 10569 | CB | CYS | 1579 | 17.268 -18.119 | -3.256 | 1.00 18.58 |
| MOTA | 10570 | SG | CYS | 1579 | 17.273 -16.870 | -1.911 | 1.00 20.66 |
| ATOM | 10571 | c | CYS | 1579 | 18.550 -19.569 | -1.708 | 1.00 16.46 |
| ATOM | 10572 | o | CYS | 1579 | 18.254 -19.737 | -0.523 | 1.00 16.94 |
| MOTA | 10572 | N | LEU | 1580 | 19.797 -19.406 | -2.127 | 1.00 16.30 |
| ATOM | 10574 | CA | LEU | 1580 | 20.901 -19.306 | -1.183 | 1.00 16.34 |
| | | | | | 22.225 -19.741 | -1.183 | 1.00 16.34 |
| ATOM | 10575 | CB | LEU | 1580 | | | |
| ATOM | 10576 | CG | LEU | 1580 | 23.496 -19.451 | -1.005 | 1.00 16.78 |
| MOTA | 10577 | CDI | LEU | 1580 | 23.455 -20.123 | 0.360 | 1.00 18.05 |

| ATOM | 10578 | CD2 | LEU | 1580 | 24.697 | -19.931 | -1.797 | 1.00 19.94 |
|--------------|-------|-----|-----|------|--------|---------|--------|------------|
| ATOM | 10579 | C | LEU | 1580 | | -17.803 | -0.914 | 1.00 16.05 |
| ATOM | 10580 | Ö | LEU | 1580 | | -16.998 | -1.813 | 1.00 13.83 |
| MOTA | 10581 | N | LEU | 1581 | | -17.437 | 0.321 | 1.00 16.04 |
| ATOM | 10582 | CA | LEU | 1581 | | -16.039 | 0.704 | 1.00 15.99 |
| | | | LEU | 1581 | | -15.812 | 1.472 | 1.00 16.23 |
| ATOM | 10583 | CB | | | | -14.413 | 1.600 | 1.00 10.25 |
| MOTA | 10584 | CG | LEU | 1581 | | | | |
| MOTA | 10585 | | LEU | 1581 | | -14.552 | 2.230 | 1.00 16.42 |
| MOTA | 10586 | | LEU | 1581 | | -13.487 | 2.444 | 1.00 19.60 |
| MOTA | 10587 | С | LEU | 1581 | | -15.583 | 1.569 | 1.00 16.66 |
| MOTA | 10588 | 0 | LEU | 1581 | | -16.063 | 2.684 | 1.00 15.52 |
| MOTA | 10589 | N | LEU | 1582 | | -14.679 | 1.032 | 1.00 15.45 |
| MOTA | 10590 | CA | LEU | 1582 | | -14.105 | 1.761 | 1.00 16.37 |
| MOTA | 10591 | CB | LEU | 1582 | 24.732 | -13.839 | 0.850 | 1.00 17.30 |
| MOTA | 10592 | CG | LEU | 1582 | 25.836 | -14.894 | 0.746 | 1.00 18.08 |
| MOTA | 10593 | CD1 | LEU | 1582 | 25.274 | -16.177 | 0.172 | 1.00 19.04 |
| MOTA | 10594 | CD2 | LEU | 1582 | 26.966 | -14.348 | -0.130 | 1.00 20.45 |
| ATOM | 10595 | С | LEU | 1582 | 23.032 | -12.769 | 2.290 | 1.00 16.32 |
| ATOM | 10596 | 0 | LEU | 1582 | | -12.046 | 1.593 | 1.00 18.36 |
| ATOM | 10597 | N | ALA | 1583 | | -12.447 | 3.521 | 1.00 15.51 |
| ATOM | 10598 | CA | ALA | 1583 | | -11.183 | 4.111 | 1.00 14.69 |
| ATOM | 10599 | CB | ALA | 1583 | | -11.416 | 5.219 | 1.00 14.69 |
| ATOM | 10600 | C | ALA | 1583 | | -10.491 | 4.667 | 1.00 14.14 |
| ATOM | 10601 | 0 | ALA | 1583 | | -11.112 | 5.344 | 1.00 13.73 |
| | 10601 | N | ASP | 1584 | 24.376 | -9.207 | 4.362 | 1.00 13.75 |
| MOTA | | | | 1584 | 25.505 | -8.429 | 4.855 | 1.00 14.49 |
| ATOM | 10603 | CA | ASP | 1584 | | | 4.091 | 1.00 15.94 |
| MOTA | 10604 | CB | ASP | | 25.647 | -7.117 | | 1.00 13.34 |
| MOTA | 10605 | CG | ASP | 1584 | 26.458 | -7.241 | 2.830 | |
| MOTA | 10606 | | ASP | 1584 | 27.193 | -8.226 | 2.661 | 1.00 20.03 |
| ATOM | 10607 | | ASP | 1584 | 26.357 | -6.311 | 2.006 | 1.00 18.72 |
| MOTA | 10608 | С | ASP | 1584 | 25.332 | -8.032 | 6.304 | 1.00 13.45 |
| MOTA | 10609 | 0 | ASP | 1584 | 24.219 | -7.753 | 6.739 | 1.00 12.56 |
| MOTA | 10610 | N | LEU | 1585 | 26.427 | -8.040 | | 1.00 12.65 |
| MOTA | 10611 | CA | LEU | 1585 | 26.381 | -7.514 | 8.410 | 1.00 13.11 |
| MOTA | 10612 | CB | LEU | 1585 | 27.360 | -8.227 | 9.356 | 1.00 13.48 |
| ATOM | 10613 | CG | LEU | 1585 | 26.969 | -9.646 | 9.777 | 1.00 13.68 |
| ATOM | 10614 | CD1 | LEU | 1585 | 27.863 | -10.134 | 10.933 | 1.00 12.03 |
| ATOM | 10615 | CD2 | LEU | 1585 | 25.504 | -9.664 | 10.207 | 1.00 14.07 |
| MOTA | 10616 | С | LEU | 1585 | 26.877 | -6.102 | 8.080 | 1.00 15.51 |
| ATOM | 10617 | 0 | LEU | 1585 | 27.954 | -5.926 | 7.483 | 1.00 15.43 |
| ATOM | 10618 | N | PRO | 1586 | 26.083 | -5.082 | 8.422 | 1.00 14.53 |
| ATOM | 10619 | CD | PRO | 1586 | 24.747 | -5.205 | 9.030 | 1.00 16.55 |
| ATOM | 10620 | CA | PRO | 1586 | 26.413 | -3.681 | 8.163 | 1.00 14.80 |
| ATOM | 10621 | CB | PRO | 1586 | 25.078 | -2.974 | 8.385 | 1.00 14.42 |
| ATOM | 10622 | CG | PRO | 1586 | 24.459 | -3.794 | 9.483 | 1.00 15.58 |
| ATOM | 10623 | c | PRO | 1586 | 27.540 | -3.066 | 8.993 | 1.00 15.36 |
| ATOM | 10624 | ō | PRO | 1586 | 28.135 | -3.709 | 9.864 | 1.00 13.48 |
| ATOM | 10625 | N | PHE | 1587 | 27.808 | -1.799 | 8.695 | 1.00 13.29 |
| ATOM | 10626 | CA | PHE | 1587 | 28.831 | -1.006 | 9.359 | 1.00 15.40 |
| ATOM | 10627 | CB | PHE | 1587 | 28.626 | 0.466 | 8.995 | 1.00 15.27 |
| | | CG | PHE | 1587 | 29.456 | 1.415 | 9.808 | 1.00 16.43 |
| MOTA MOTA | 10628 | CD1 | | | 30.845 | 1.346 | 9.776 | |
| | 10629 | | | 1587 | 28.848 | 2.378 | 10.610 | 1.00 15.31 |
| ATOM | 10630 | - | PHE | | | 2.215 | 10.533 | 1.00 10.01 |
| MOTA | 10631 | | PHE | 1587 | 31.619 | | | 1.00 19.00 |
| ATOM | 10632 | | PHE | 1587 | 29.619 | 3.257 | 11.374 | 1.00 18.40 |
| MOTA | 10633 | CZ | PHE | 1587 | 31.009 | 3.174 | 11.332 | |
| ATOM | 10634 | С | PHE | 1587 | 28.804 | -1.176 | 10.875 | 1.00 14.93 |
| ATOM | 10635 | 0 | PHE | 1587 | 27.783 | -0.954 | 11.513 | 1.00 13.77 |
| MOTA | 10636 | N | MET | 1588 | 29.944 | -1.580 | 11.431 | 1.00 16.41 |
| MOTA | 10637 | CA | MET | 1588 | 30.115 | -1.783 | 12.866 | 1.00 15.60 |
| MOTA | 10638 | CB | MET | 1588 | 29.958 | -0.452 | 13.610 | 1.00 15.47 |
| MOTA | 10639 | CG | MET | 1588 | 30.753 | -0.398 | 14.899 | 1.00 17.28 |
| ATOM | 10640 | SD | MET | 1588 | 32.552 | -0.481 | 14.654 | 1.00 16.90 |
| MOTA | 10641 | CE | MET | 1588 | 32.900 | 1.224 | 14.358 | 1.00 19.88 |
| MOTA | 10642 | C | MET | 1588 | 29.182 | -2.825 | 13.480 | 1.00 14.81 |
| MOTA | 10643 | 0 | MET | 1588 | 28.832 | -2.742 | 14.659 | 1.00 16.79 |
| ATOM | 10644 | N | ALA | 1589 | 28.782 | -3.809 | 12.689 | 1.00 13.82 |
| MOTA | 10645 | CA | ALA | 1589 | 27.901 | -4.853 | 13.196 | 1.00 14.09 |
| ATOM | 10646 | CB | ALA | 1589 | 26.873 | -5.228 | 12.123 | 1.00 14.61 |
| ATOM | 10647 | С | ALA | 1589 | 28.707 | -6.079 | 13.617 | 1.00 14.92 |
| MOTA | 10648 | 0 | ALA | 1589 | 28.148 | -7.055 | 14.116 | 1.00 17.78 |
| ATOM | 10649 | N | TYR | 1590 | 30.024 | -6.023 | 13.421 | 1.00 14.09 |
| ATOM | 10650 | CA | TYR | 1590 | 30.911 | -7.130 | 13.775 | 1.00 15.98 |
| ATOM | 10651 | CB | TYR | 1590 | 31.164 | -8.010 | 12.543 | 1.00 16.40 |
| ATOM | 10652 | CG | TYR | 1590 | 31.512 | -7.250 | 11.277 | 1.00 15.39 |
| ATOM | 10653 | CD1 | | 1590 | 32.816 | -7.232 | 10.783 | 1.00 13.60 |
| ATOM | 10654 | CE1 | TYR | 1590 | 33.127 | -6.558 | 9.596 | 1.00 15.26 |
| | | | | | | | | |

| ATOM | 10655 | CD2 | TYR | 1590 | 30.524 | -6.571 | 10.559 | 1.00 14.4 |
|------|-------|-----|------|------|--------|---------|--------|-----------|
| ATOM | 10656 | CE2 | TYR | 1590 | 30.818 | -5.895 | 9.378 | 1.00 14.9 |
| ATOM | 10657 | cz | TYR | 1590 | 32.118 | -5.895 | 8.901 | 1.00 14.5 |
| ATOM | 10658 | OH | TYR | 1590 | 32.380 | -5.247 | 7.718 | 1.00 14.9 |
| ATOM | 10659 | С | TYR | 1590 | 32.225 | -6.601 | 14.334 | 1.00 16.9 |
| ATOM | 10660 | 0 | TYR | 1590 | 33.303 | -7.077 | 13.980 | 1.00 17.1 |
| ATOM | 10661 | N | ALA | 1591 | 32.109 | -5.626 | 15.235 | 1.00 16.9 |
| ATOM | 10662 | CA | ALA | 1591 | 33.257 | -4.973 | 15.863 | 1.00 18.1 |
| ATOM | 10663 | CB | ALA | 1591 | 32.790 | -3.734 | 16.617 | 1.00 16.8 |
| ATOM | 10664 | C | ALA | 1591 | 34.012 | -5.909 | 16.798 | 1.00 17.7 |
| ATOM | 10665 | 0 | ALA | 1591 | 35.212 | -5.759 | 17.005 | 1.00 16.3 |
| MOTA | 10666 | N | THR | 1592 | 33.289 | -6.868 | 17.366 | 1.00 17.8 |
| ATOM | 10667 | CA | THR | 1592 | 33.871 | -7.863 | 18.254 | 1.00 17.1 |
| ATOM | 10668 | СВ | THR | 1592 | 33.583 | -7.570 | 19.739 | 1.00 17.5 |
| ATOM | 10669 | OG1 | THR | 1592 | 32.176 | -7.682 | 19.991 | 1.00 16.8 |
| ATOM | 10670 | CG2 | THR | 1592 | 34.059 | -6.169 | 20.112 | 1.00 16.1 |
| ATOM | 10671 | C | THR | 1592 | 33.208 | -9.184 | 17.900 | 1.00 15.8 |
| ATOM | 10672 | 0 | THR | 1592 | 32.114 | -9.201 | 17.329 | 1.00 13.6 |
| ATOM | 10672 | N | PRO | 1593 | | -10.310 | 18.223 | 1.00 16.0 |
| | 10674 | | PRO | 1593 | | -10.310 | 18.675 | 1.00 16.8 |
| ATOM | | CD | | 1593 | | -10.403 | 17.903 | 1.00 16.0 |
| MOTA | 10675 | CA | PRO | | | | | 1.00 10.0 |
| ATOM | 10676 | CB | PRO | 1593 | | -12.599 | 18.459 | 1.00 17.7 |
| ATOM | 10677 | CG | PRO | 1593 | | -11.877 | 18.233 | |
| ATOM | 10678 | С | PRO | 1593 | | -11.769 | 18.531 | 1.00 16.8 |
| ATOM | 10679 | 0 | PRO | 1593 | | -12.190 | 17.858 | 1.00 15.9 |
| ATOM | 10680 | N | GLU | 1594 | | -11.417 | 19.810 | 1.00 17.1 |
| MOTA | 10681 | CA | GLU | 1594 | | -11.548 | 20.507 | 1.00 17.8 |
| MOTA | 10682 | CB | GLU | 1594 | | -11.095 | 21.966 | 1.00 21.8 |
| MOTA | 10683 | CG | GLU | 1594 | | -11.407 | 22.830 | 1.00 29.0 |
| MOTA | 10684 | CD | GLU. | 1594 | | -11.163 | 24.308 | 1.00 34.9 |
| ATOM | 10685 | OE1 | GLU | 1594 | 30.087 | -10.036 | 24.649 | 1.00 37.1 |
| MOTA | 10686 | OE2 | GLU | 1594 | 29.429 | -12.091 | 25.124 | 1.00 37.4 |
| MOTA | 10687 | С | GLU | 1594 | 29.369 | -10.755 | 19.817 | 1.00 16.2 |
| MOTA | 10688 | 0 | GLU | 1594 | 28.233 | -11.210 | 19.721 | 1.00 14.7 |
| MOTA | 10689 | N | GLN | 1595 | 29.708 | -9.568 | 19.326 | 1.00 16.1 |
| MOTA | 10690 | CA | GLN | 1595 | 28.715 | -8.749 | 18.645 | 1.00 16.6 |
| MOTA | 10691 | CB | GLN | 1595 | 29.209 | -7.319 | 18.489 | 1.00 19.0 |
| ATOM | 10692 | CG | GLN | 1595 | 29.345 | -6.591 | 19.814 | 1.00 25.3 |
| ATOM | 10693 | CD | GLN | 1595 | 29.618 | -5.113 | 19.634 | 1.00 28.2 |
| ATOM | 10694 | | GLN | 1595 | 28.854 | -4.411 | 18.974 | 1.00 30.7 |
| ATOM | 10695 | NE2 | | 1595 | 30.709 | -4.629 | 20.228 | 1.00 31.6 |
| ATOM | 10696 | C | GLN | 1595 | 28.401 | -9.344 | 17.282 | 1.00 13.9 |
| MOTA | 10697 | ō | GLN | 1595 | 27.261 | -9.290 | 16.826 | 1.00 12.9 |
| ATOM | 10698 | N | ALA | 1596 | 29.410 | -9.918 | 16.636 | 1.00 12.1 |
| MOTA | 10699 | CA | ALA | 1596 | | -10.530 | 15.339 | 1.00 12.3 |
| ATOM | 10700 | СВ | ALA | 1596 | | -10.993 | 14.730 | 1.00 11.0 |
| ATOM | 10701 | C | ALA | 1596 | 28.212 | -11.702 | 15.484 | 1.00 12.0 |
| ATOM | 10702 | ō | ALA | 1596 | 27.345 | -11.897 | 14.632 | 1.00 11.8 |
| ATOM | 10703 | N | PHE | 1597 | | -12.470 | 16.566 | 1.00 13.2 |
| ATOM | 10704 | CA | PHE | 1597 | | -13.630 | 16.787 | 1.00 12.2 |
| ATOM | 10705 | CB | PHE | 1597 | | -14.392 | 18.077 | 1.00 11.3 |
| ATOM | 10706 | CG | PHE | 1597 | - | -14.829 | 18.165 | 1.00 12.7 |
| ATOM | 10707 | | PHE | 1597 | | -15.142 | 17.018 | 1.00 14.7 |
| ATOM | 10707 | | PHE | 1597 | | -14.963 | 19.406 | 1.00 13.5 |
| ATOM | 10709 | | PHE | 1597 | | -15.586 | 17.107 | 1.00 15.5 |
| ATOM | 10710 | | PHE | 1597 | | -15.407 | 19.513 | 1.00 13.4 |
| | 10711 | CZ | PHE | 1597 | | -15.718 | 18.354 | 1.00 15.9 |
| MOTA | 10711 | C | PHE | 1597 | | -13.716 | 16.912 | 1.00 13.5 |
| MOTA | | | | | | | | 1.00 12.3 |
| MOTA | 10713 | 0 | PHE | 1597 | | -13.834 | 16.346 | |
| ATOM | 10714 | N | GLU | 1598 | | -12.134 | 17.667 | 1.00 12.5 |
| ATOM | 10715 | CA | GLU | 1598 | | -11.641 | 17.892 | 1.00 13.4 |
| MOTA | 10716 | CB | GLU | 1598 | | -10.541 | 18.955 | 1.00 16.3 |
| ATOM | 10717 | CG | GLU | 1598 | | -10.001 | 19.313 | 1.00 23.4 |
| ATOM | 10718 | CD | GLU | 1598 | | -10.950 | 20.189 | 1.00 28.9 |
| MOTA | 10719 | | GLU | 1598 | | -12.188 | 20.109 | 1.00 31.0 |
| ATOM | 10720 | | GLU | 1598 | | -10.452 | 20.953 | 1.00 32.0 |
| MOTA | 10721 | С | GLU | 1598 | | -11.113 | 16.615 | 1.00 12.7 |
| MOTA | 10722 | 0 | GLU | 1598 | 22.634 | -11.425 | 16.321 | 1.00 11.2 |
| MOTA | 10723 | N | ASN | 1599 | | -10.316 | 15.852 | 1.00 12.0 |
| MOTA | 10724 | CA | ASN | 1599 | 23.953 | -9.758 | 14.640 | 1.00 11.5 |
| MOTA | 10725 | CB | ASN | 1599 | 24.740 | -8.513 | 14.228 | 1.00 12.9 |
| MOTA | 10726 | CG | ASN | 1599 | 24.671 | -7.422 | 15.295 | 1.00 13.2 |
| MOTA | 10727 | OD1 | ASN | 1599 | 23.617 | -7.218 | 15.908 | 1.00 13.3 |
| MOTA | 10728 | ND2 | ASN | 1599 | 25.774 | -6.712 | 15.510 | 1.00 13.7 |
| MOTA | 10729 | C | ASN | 1599 | 23.865 | -10.771 | 13.507 | 1.00 11.8 |
| MOTA | 10730 | 0 | ASN | 1599 | | -10.696 | 12.677 | 1.00 11.9 |
| MOTA | 10731 | N | ALA | 1600 | 24.790 | -11.724 | 13.471 | 1.00 9.5 |

| ATOM | 10732 | CA | ALA | 1600 | 24.732 -12.754 | 12.440 | 1.00 11.81 |
|--------------|----------------|--------|------------|--------------|----------------------------------|--------|--------------------------|
| MOTA | 10733 | CB | ALA | 1600 | 25.994 -13.610 | 12.462 | 1.00 11.15 |
| ATOM | 10734 | С | ALA | 1600 | 23.503 -13.615 | | 1.00 11.76 |
| MOTA | 10735 | 0 | ALA | 1600 | 22.763 -13.990 | 11.838 | 1.00 12.58 |
| ATOM | 10736 | N | ALA | 1601 | 23.283 -13.922 | 14.019 | 1.00 11.05 |
| ATOM | 10737 | CA | ALA | 1601 | 22.142 -14.746 | 14.391 | 1.00 11.07 |
| ATOM | 10738 | CB | ALA | 1601 | 22.183 -15.080 | 15.889 | 1.00 12.88 |
| MOTA | 10739 | C | ALA | 1601 | 20.830 -14.051 | 14.038 | 1.00 11.65 |
| ATOM | 10740 | 0 | ALA | 1601 | 19.868 -14.700 | 13.624 | 1.00 12.48 |
| ATOM | 10741 | N | THR | 1602 | 20.782 -12.735 | 14.198 | 1.00 10.09 |
| ATOM | 10742 | CA | THR | 1602 | 19.565 -11.980 | 13.884 | 1.00 10.55 |
| MOTA | 10743 | CB | THR | 1602 | 19.718 -10.486 | 14.224 | 1.00 10.24 |
| ATOM | 10744 | OG1 | THR | 1602 | 19.875 -10.342 | 15.638 | 1.00 12.17 |
| ATOM | 10745 | CG2 | THR | 1602 | 18.491 -9.703 | | 1.00 11.96 |
| ATOM | 10746 | C | THR | 1602 | 19.211 -12.089 | 12.408 | 1.00 11.71 |
| MOTA | 10747 | 0 | THR | 1602 | 18.060 -12.356 | | 1.00 10.21 |
| MOTA | 10748 | N | VAL | 1603 | 20.193 -11.884 | | 1.00 8.99 |
| MOTA | 10749 | CA | VAL | 1603 | 19.897 -11.956 | | 1.00 10.74 |
| MOTA | 10750 | CB | VAL | 1603 | 20.997 -11.276 | | 1.00 12.65 |
| MOTA | 10751 | | VAL | 1603 | 20.519 -11.129 | | 1.00 19.78 |
| MOTA | 10752 | | VAL | 1603 | 21.309 -9.885 | | 1.00 13.29 |
| ATOM | 10753 | C | VAL | 1603 | 19.679 -13.401 | | 1.00 10.88 |
| ATOM | 10754 | 0 | VAL | 1603 | 18.931 -13.651 | | 1.00 11.56 |
| MOTA | 10755 | N | MET | 1604 | 20.322 -14.354 | | 1.00 10.50 |
| MOTA | 10756 | CA | MET | 1604 | 20.118 -15.768 | | 1.00 11.08 |
| ATOM | 10757 | CB | MET | 1604 | 21.082 -16.672 | | 1.00 15.41 |
| ATOM | 10758 | CG | MET | 1604 | 22.562 -16.538 | | 1.00 18.50 |
| MOTA | 10759 | SD | MET | 1604 | 22.958 -17.034 | | 1.00 27.30 |
| ATOM | | CE | MET | 1604 | 22.871 -18.884 | | 1.00 21.09 |
| MOTA | 10761 | C | MET | 1604 | 18.677 -16.169 | | 1.00 10.81 |
| MOTA | 10762 | 0 | MET | 1604 | 17.984 -16.794 | | 1.00 13.07 |
| MOTA | 10763 | N | ARG | 1605 | 18.222 -15.811 | | 1.00 11.02 |
| MOTA | 10764 | CA | ARG | 1605 | 16.861 -16.158 | | 1.00 12.52 |
| ATOM | 10765 | CB | ARG | 1605 | 16.582 -15.724 | | 1.00 13.71 |
| MOTA | 10766 | CG | ARG | 1605 | 17.431 -16.445 | | 1.00 13.88 |
| ATOM | 10767 | CD | ARG | 1605 | 16.798 -16.395 | | 1.00 14.01 |
| MOTA | 10768 | NE | ARG | 1605 | 17.771 -16.750 | | 1.00 18.79 |
| MOTA | 10769 | CZ | ARG | 1605 | 18.649 -15.898 | | 1.00 18.25 |
| MOTA | 10770 | NH1 | | 1605 | 18.670 -14.636 | | 1.00 18.55 |
| ATOM | 10771 | NH2 | | 1605 | 19.521 -16.314 | | 1.00 18.62 |
| ATOM | 10772 | С | ARG | 1605 | 15.814 -15.534 | | 1.00 12.91 |
| ATOM | 10773 | 0 | ARG | 1605 | 14.724 -16.090 | | 1.00 12.21 1.00 11.94 |
| ATOM | 10774 | N | ALA | 1606 | 16.141 -14.386 | | 1.00 11.94 |
| ATOM | 10775 | CA | ALA | 1606 | 15.223 -13.704 15.632 -12.232 | • | 1.00 12.22 |
| ATOM | 10776 | СВ | ALA | 1606 | 15.632 -12.232 15.136 -14.374 | | 1.00 11.74 |
| ATOM | 10777 10778 | С 0 | ALA ALA | 1606 1606 | 14.274 -14.021 | | 1.00 13.10 |
| ATOM ATOM | 10778 | N | GLY | 1607 | 16.023 -15.331 | | 1.00 14.17 |
| ATOM | 10779 | CA | GLY | 1607 | 15.980 -16.029 | | 1.00 12.33 |
| ATOM | 10781 | CA | GLY | 1607 | 17.288 -16.273 | | 1.00 11.83 |
| ATOM | 10781 | 0 | GLY | 1607 | 17.316 -17.063 | | 1.00 15.36 |
| ATOM | 10782 | N | ALA | 1607 | 18.368 ÷15.612 | | 1.00 13.30 |
| ATOM | 10784 | CA | ALA | 1608 | 19.668 -15.767 | | 1.00 11.14 |
| ATOM | 10785 | CB | ALA | 1608 | 20.621 -14.689 | | 1.00 13.69 |
| ATOM | 10785 | СВ | ALA | 1608 | 20.294 -17.153 | | 1.00 13.84 |
| ATOM | 10787 | o | ALA | 1608 | 20.234 -17.799 | | 1.00 11.53 |
| ATOM | 10788 | N | ASN | 1609 | 21.135 -17.602 | | 1.00 13.34 |
| ATOM | 10789 | CA | ASN | 1609 | 21.814 -18.895 | | 1.00 13.10 |
| MOTA | 10790 | CB | ASN | 1609 | 21.736 -19.734 | | 1.00 14.21 |
| ATOM | 10791 | CG | ASN | 1609 | 20.321 -20.082 | | 1.00 15.93 |
| ATOM | 10792 | OD1 | | 1609 | 19.606 -20.775 | | 1.00 18.98 |
| ATOM | 10793 | ND2 | | 1609 | 19.910 -19.610 | | 1.00 12.95 |
| ATOM | 10794 | С | ASN | 1609 | 23.293 -18.648 | | 1.00 14.73 |
| ATOM | 10795 | ō | ASN | 1609 | 24.021 -19.533 | | 1.00 15.75 |
| ATOM | 10796 | N | MET | 1610 | 23.732 -17.435 | | 1.00 13.00 |
| ATOM | 10797 | CA | MET | 1610 | 25.132 -17.083 | | 1.00 13.92 |
| ATOM | 10798 | СВ | MET | 1610 | 25.864 -17.514 | | 1.00 14.99 |
| ATOM | 10799 | CG | MET | 1610 | 27.293 -17.047 | | 1.00 18.34 |
| ATOM | 10800 | SD | MET | 1610 | 27.934 -17.568 | | 1.00 19.59 |
| ATOM | 10801 | CE | MET | 1610 | 28.973 -18.934 | | 1.00 21.61 |
| ATOM | 10802 | C | MET | 1610 | 25.270 -15.586 | | 1.00 13.22 |
| ATOM | 10803 | ō | MET | 1610 | 24.400 -14.808 | | 1.00 12.57 |
| ATOM | 10804 | N | VAL | 1611 | 26.366 -15.185 | | 1.00 13.16 |
| ATOM | 10805 | CA | VAL | 1611 | 26.603 -13.782 | | 1.00 14.59 |
| MOTA | 10806 | CB | VAL | 1611 | 26.750 -13.580 | 7.859 | 1.00 18.07 |
| MOTA | 10807 | | VAL | 1611 | 27.320 -12.237 | | 1.00 23.20 |
| MOTA | 10808 | | VAL | 1611 | 25.389 -13.741 | | 1.00 17.45 |
| | | | | | | | |

| MOTA | 10809 | С | VAL | 1611 | 27.853 - | -13 289 | 5.621 | 1.00 15.11 | |
|---|--|---|--|--|--|--|--|--|---|
| | | | | | | | | | |
| MOTA | 10810 | 0 | VAL | 1611 | 28.844 - | | 5.518 | 1.00 13.59 | |
| MOTA | 10811 | N | LYS | 1612 | 27.797 - | -12.061 | 5.108 | 1.00 13.93 | |
| MOTA | 10812 | CA | LYS | 1612 | 28.942 - | -11.471 | 4.420 | 1.00 13.65 | |
| ATOM | 10813 | CB | LYS | 1612 | 28.541 - | | 3.023 | 1.00 16.26 | |
| | | | | | | | | | |
| ATOM | 10814 | CG | LYS | 1612 | 29.718 - | | 2.207 | 1.00 16.17 | |
| ATOM | 10815 | CD | LYS | 1612 | 29.419 - | -10.402 | 0.703 | 1.00 19.74 | |
| ATOM | 10816 | CE | LYS | 1612 | 28.447 | -9.294 | 0.338 | 1.00 20.53 | |
| | 10817 | NZ | LYS | 1612 | 29.054 | -7.938 | 0.547 | 1.00 18.43 | |
| ATOM | | | | | | | | | |
| MOTA | 10818 | С | LYS | 1612 | 29.476 - | -10.307 | 5.239 | 1.00 14.73 | |
| MOTA | 10819 | 0 | LYS | 1612 | 28.709 | -9.454 | 5.680 | 1.00 15.46 | |
| ATOM | 10820 | N | ILE | 1613 | 30.792 - | -10.280 | 5.439 | 1.00 15.79 | |
| | | | | | | | | | |
| ATOM | 10821 | CA | ILE | 1613 | 31.436 | -9.215 | 6.210 | 1.00 17.39 | |
| ATOM | 10822 | CB | ILE | 1613 | 31.868 | -9.699 | 7.623 | 1.00 17.61 | |
| ATOM | 10823 | CG2 | ILE | 1613 | 30.642 | -9.920 | 8.507 | 1.00 18.44 | |
| MOTA | 10824 | CG1 | TLE | 1613 | 32.706 - | | 7.502 | 1.00 18.71 | |
| | | | | | | | | | |
| MOTA | 10825 | CD1 | | 1613 | 33.102 - | | 8.835 | 1.00 21.00 | |
| MOTA | 10826 | С | ILE | 1613 | 32.674 | -8.698 | 5.487 | 1.00 17.52 | |
| MOTA | 10827 | 0 | ILE | 1613 | 33.363 | -9.453 | 4.805 | 1.00 17.34 | |
| MOTA | 10828 | N | GLU | 1614 | 32.948 | -7.410 | 5.658 | 1.00 18.44 | |
| | | | | | | | | | |
| MOTA | 10829 | | GLU | 1614 | 34.077 | -6.756 | 5.014 | 1.00 22.04 | |
| ATOM | 10830 | CB | GLU | 1614 | 33.699 | -5.319 | 4.650 | 1.00 21.72 | |
| MOTA | 10831 | CG | GLU | 1614 | 32.556 | -5.213 | 3.663 | 1.00 24.57 | |
| ATOM | 10832 | CD | GLU | 1614 | 32.210 | -3.773 | 3.316 | 1.00 25.01 | |
| | | | | | | | | | |
| MOTA | 10833 | OE1 | | 1614 | 33.048 | -2.879 | 3.551 | 1.00 25.95 | |
| ATOM | 10834 | OE2 | GLU | 1614 | 31.103 | -3.535 | 2.793 | 1.00 26.44 | |
| MOTA | 10835 | С | GLU | 1614 | 35.330 | -6.730 | 5.879 | 1.00 22.81 | |
| MOTA | 10836 | | GLU | 1614 | 35.270 | -6.387 | | 1.00 23.72 | |
| | | | | | | | | | |
| ATOM | 10837 | | GLY | 1615 | | -7.082 | 5.292 | 1.00 24.76 | |
| ATOM | 10838 | CA | GLY | 1615 | 37.706 | -7.063 | 6.052 | 1.00 26.31 | |
| ATOM | 10839 | C | GLY | 1615 | 38.657 | -8.191 | 5.724 | 1.00 25.48 | |
| ATOM | 10840 | | | 1615 | 38.264 | -9.195 | 5.132 | 1.00 26.13 | |
| | | | | | | | | | |
| MOTA | 10841 | | GLY | 1616 | 39.916 | -8.024 | 6.117 | 1.00 26.28 | |
| ATOM | 10842 | CA | GLY | 1616 | 40.917 | -9.043 | 5.855 | 1.00 25.88 | |
| ATOM | 10843 | С | GLY | 1616 | 41.395 | -9.771 | 7.101 | 1.00 26.83 | |
| ATOM | 10844 | | GLY | 1616 | 40.592 - | | 7.862 | 1.00 26.50 | |
| | | | | | | | | | |
| MOTA | 10845 | | GLU | 1617 | 42.712 | -9.780 | 7.293 | 1.00 23.60 | |
| MOTA | 10846 | CA | GLU | 1617 | 43.369 - | -10.427 | 8.427 | 1.00 25.78 | |
| MOTA | 10847 | CB | GLU | 1617 | 44.811 | -9.923 | 8.554 | 1.00 28.43 | |
| MOTA | 10848 | | GLU | 1617 | 45.856 - | | 7.868 | 1.00 35.94 | |
| | | | | | | | | | |
| ATOM | 10849 | | GLU | 1617 | 46.136 - | | 8.604 | 1.00 39.30 | |
| MOTA | 10850 | OE1 | GLU | 1617 | 45.199 - | -12.883 | 8.770 | 1.00 39.90 | |
| N/IIOM | | | | | | | | | |
| ATOM | 10851 | OE2 | GLU | 1617 | 47.299 - | -12.283 | | | |
| MOTA MOTA | 10851 | OE2 | | 1617 1617 | 47.299 - 42.718 - | | 9.015 | 1.00 39.51 | |
| MOTA | 10852 | С | GLU | 1617 | 42.718 - | 10.294 | 9.015 9.800 | 1.00 39.51 1.00 23.15 | |
| MOTA MOTA | 10852 10853 | C O | GLU GLU | 1617 1617 | 42.718 - 42.527 - | -10.294 -11.289 | 9.015 9.800 10.499 | 1.00 39.51 1.00 23.15 1.00 24.44 | |
| MOTA | 10852 | C O | GLU | 1617 | 42.718 - | 10.294 | 9.015 9.800 10.499 10.202 | 1.00 39.51 1.00 23.15 | |
| MOTA MOTA | 10852 10853 | C O N | GLU GLU | 1617 1617 | 42.718 - 42.527 - | -10.294 -11.289 | 9.015 9.800 10.499 | 1.00 39.51 1.00 23.15 1.00 24.44 | |
| MOTA MOTA MOTA | 10852 10853 10854 10855 | C O N CA | GLU GLU TRP TRP | 1617 1617 1618 1618 | 42.718 - 42.527 - 42.404 41.830 | -10.294 -11.289 -9.069 -8.855 | 9.015 9.800 10.499 10.202 11.518 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 20.46 | |
| ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 | C O N CA CB | GLU GLU TRP TRP TRP | 1617 1617 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 | -10.294 -11.289 -9.069 -8.855 -7.364 | 9.015 9.800 10.499 10.202 11.518 11.776 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 20.46 1.00 21.59 | |
| MOTA MOTA MOTA MOTA MOTA MOTA MOTA | 10852 10853 10854 10855 10856 10857 | C O N CA CB | GLU GLU TRP TRP TRP TRP | 1617 1617 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 20.46 1.00 21.59 1.00 19.95 | |
| MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA | 10852 10853 10854 10855 10856 10857 10858 | C O N CA CB CG CD2 | GLU GLU TRP TRP TRP TRP | 1617 1617 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 20.46 1.00 21.59 1.00 19.95 1.00 19.68 | |
| MOTA MOTA MOTA MOTA MOTA MOTA MOTA | 10852 10853 10854 10855 10856 10857 | C O N CA CB CG CD2 | GLU GLU TRP TRP TRP TRP | 1617 1617 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 20.46 1.00 21.59 1.00 19.95 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10859 | C O N CA CB CG CD2 CE2 | GLU GLU TRP TRP TRP TRP TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 20.46 1.00 21.59 1.00 19.95 1.00 19.68 1.00 17.75 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10859 10860 | C O N CA CB CG CD2 CE2 CE3 | GLU GLU TRP TRP TRP TRP TRP TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 20.46 1.00 21.59 1.00 19.95 1.00 19.68 1.00 17.75 1.00 18.42 | _ |
| MOTA ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10859 10860 10861 | C O N CA CB CG CD2 CE2 CE3 CD1 | GLU GLU TRP TRP TRP TRP TRP TRP TRP TRP | 1617 1618 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 | - |
| MOTA ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10859 10860 10861 10862 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 | GLU GLU TRP TRP TRP TRP TRP TRP TRP TRP TRP | 1617 1618 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.845 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 | - |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10859 10860 10861 10862 10863 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.845 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.95 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 | - |
| MOTA ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10859 10860 10861 10862 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 | GLU GLU TRP TRP TRP TRP TRP TRP TRP TRP TRP | 1617 1618 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.845 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10859 10860 10861 10862 10863 10864 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.845 -5.557 -6.345 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 20.46 1.00 21.59 1.00 19.95 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 19.55 1.00 19.55 1.00 19.55 | • |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10859 10860 10861 10862 10863 10864 10865 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 CH2 | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.845 -5.557 -6.345 -5.771 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 20.46 1.00 21.59 1.00 19.95 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 18.71 1.00 19.07 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10859 10860 10861 10862 10863 10864 10865 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 CH2 C | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.845 -5.557 -6.345 -5.771 -9.619 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 20.46 1.00 21.59 1.00 19.95 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 18.71 1.00 19.07 1.00 20.59 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10859 10860 10861 10862 10863 10864 10865 10866 10867 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 CH2 C | GLU GLU TRP | 1617 1618 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.845 -5.557 -6.557 -7.1 -9.619 -9.746 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 19.57 1.00 19.77 1.00 19.07 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10859 10860 10861 10862 10863 10864 10865 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 CH2 C | GLU GLU TRP | 1617 1618 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.845 -5.557 -6.557 -7.1 -9.619 -9.746 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 20.46 1.00 21.59 1.00 19.95 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 18.71 1.00 19.07 1.00 20.59 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10860 10861 10862 10863 10864 10865 10866 10867 10868 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 CH2 CO N | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.845 -5.557 -6.345 -5.771 -9.746 10.144 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 19.57 1.00 19.77 1.00 19.07 | - |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10860 10861 10862 10863 10864 10865 10866 10867 10868 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 CH2 C O N CA | GLU GLU TRP | 1617 1618 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.345 -5.557 -6.345 -5.771 -9.619 -9.746 10.144 10.886 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 20.46 1.00 19.95 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 18.71 1.00 19.07 1.00 20.59 1.00 21.43 1.00 20.49 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10859 10860 10861 10862 10863 10864 10865 10866 10865 10867 10868 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 CH2 C O N CA CB | GLU GLU TRP | 1617 1618 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.845 -5.557 -6.345 -9.619 -9.746 10.886 10.622 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.696 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 20.46 1.00 21.59 1.00 19.95 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 19.55 1.00 19.55 1.00 19.07 1.00 20.59 1.00 20.59 1.00 21.43 1.00 20.49 1.00 20.97 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10857 10858 10859 10860 10861 10862 10863 10864 10865 10866 10867 10868 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 CH2 C O N CA CB CCB CC | GLU GLU TRP | 1617 1618 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - 37.106 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.845 -5.557 -6.345 -5.771 -9.619 -9.746 10.144 10.886 10.622 -9.238 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.696 9.620 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 20.46 1.00 21.59 1.00 19.95 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 19.55 1.00 19.55 1.00 19.07 1.00 20.59 1.00 21.43 1.00 21.43 1.00 20.49 1.00 20.97 1.00 20.97 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10859 10860 10861 10862 10863 10864 10865 10866 10865 10867 10868 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 CH2 C O N CA CB | GLU GLU TRP | 1617 1618 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.845 -5.557 -6.345 -9.619 -9.746 10.886 10.622 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.696 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.95 1.00 17.75 1.00 17.75 1.00 20.31 1.00 20.31 1.00 19.55 1.00 17.13 1.00 18.71 1.00 19.07 1.00 20.59 1.00 20.49 1.00 20.49 1.00 20.97 1.00 21.93 1.00 21.93 1.00 21.93 1.00 21.93 1.00 22.24 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10857 10858 10859 10860 10861 10862 10863 10864 10865 10866 10867 10868 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 CH2 C O N CA CB CCB CC | GLU GLU TRP | 1617 1618 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - 37.106 36.316 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.845 -5.557 -6.345 -5.771 -9.619 -9.746 10.144 10.886 10.622 -9.238 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.696 9.620 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 20.46 1.00 21.59 1.00 19.95 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 19.55 1.00 19.55 1.00 19.07 1.00 20.59 1.00 21.43 1.00 21.43 1.00 20.49 1.00 20.97 1.00 20.97 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10860 10861 10862 10863 10864 10865 10866 10867 10868 10870 10870 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 CH2 C O N CA CB CG CD1 CD2 | GLU GLU TRP | 1617 1618 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - 37.106 36.316 36.200 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.345 -5.557 -6.345 -5.771 -9.619 -9.746 10.144 10.886 10.622 -9.238 -9.238 -9.238 -9.39 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.696 9.696 9.696 9.8338 10.833 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 19.55 1.00 19.55 1.00 19.07 1.00 20.59 1.00 20.59 1.00 20.49 1.00 20.49 1.00 20.97 1.00 22.24 1.00 23.75 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10860 10862 10863 10864 10865 10866 10867 10868 10869 10870 10871 10872 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 CH2 C O N CA CB CG CD1 CD2 C | GLU GLU TRP | 1617 1618 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - 37.106 36.316 36.200 38.817 - | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.345 -5.557 -6.345 -5.771 -9.619 -9.746 10.144 10.886 10.622 -9.238 -9.238 -9.239 12.395 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 12.787 12.938 10.737 10.893 9.696 9.620 8.338 10.833 11.067 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.95 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 18.71 1.00 19.07 1.00 20.59 1.00 20.59 1.00 20.59 1.00 20.97 1.00 20.97 1.00 20.97 1.00 21.93 1.00 22.24 1.00 23.75 1.00 19.39 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10869 10861 10862 10863 10864 10865 10866 10866 10868 10870 10871 10872 10873 10874 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 CH2 C O N CA CB CG CD1 CD2 C O | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - 37.106 36.316 36.316 36.200 38.817 - 37.821 - | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.345 -5.557 -6.345 -5.771 -9.619 -9.746 10.886 -10.622 -9.238 -9.117 -9.039 12.395 13.094 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.696 9.620 8.338 10.833 11.067 11.238 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 20.46 1.00 19.95 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 19.55 1.00 19.55 1.00 18.71 1.00 19.57 1.00 20.59 1.00 21.43 1.00 20.49 1.00 20.97 1.00 20.97 1.00 21.93 1.00 22.24 1.00 23.75 1.00 19.39 1.00 19.39 1.00 16.11 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10860 10862 10863 10864 10865 10866 10867 10868 10869 10870 10871 10872 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 CH2 C O N CA CB CG CD1 CD2 C O | GLU GLU TRP | 1617 1618 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - 37.106 36.316 36.200 38.817 - 37.821 - 40.047 - | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.845 -5.557 -6.345 -5.771 -9.619 -9.746 10.886 10.622 -9.238 -9.117 -9.039 12.395 13.094 12.899 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.696 9.620 8.338 10.833 11.067 11.238 11.034 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.95 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 18.71 1.00 19.07 1.00 20.59 1.00 20.59 1.00 20.59 1.00 20.97 1.00 20.97 1.00 20.97 1.00 21.93 1.00 22.24 1.00 23.75 1.00 19.39 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10869 10861 10862 10863 10864 10865 10866 10866 10868 10870 10871 10872 10873 10874 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 CZ3 CH2 C O N CA CB CG CD1 CD2 C O N | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - 37.106 36.316 36.316 36.200 38.817 - 37.821 - | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.845 -5.557 -6.345 -5.771 -9.619 -9.746 10.886 10.622 -9.238 -9.117 -9.039 12.395 13.094 12.899 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.696 9.620 8.338 10.833 11.067 11.238 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 20.46 1.00 19.95 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 19.55 1.00 19.55 1.00 18.71 1.00 19.57 1.00 20.59 1.00 21.43 1.00 20.49 1.00 20.97 1.00 20.97 1.00 21.93 1.00 22.24 1.00 23.75 1.00 19.39 1.00 19.39 1.00 16.11 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10857 10858 10859 10860 10861 10863 10864 10865 10866 10867 10870 10871 10872 10873 10874 10875 10876 | C O N CA CB CG CD2 CE2 CE3 CD1 NE1 CZ2 C O N CA CB CG CD1 CD2 C O N CA CB CG CD1 CD2 C O N CA | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - 37.106 36.316 36.200 38.817 - 37.821 - 40.047 - 40.284 - | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.557 -6.345 -5.557 -6.345 -9.746 10.886 10.622 -9.238 -9.117 -9.039 12.395 12.899 14.334 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.696 9.620 8.338 10.833 11.067 11.238 11.034 11.174 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 20.46 1.00 21.59 1.00 19.95 1.00 19.68 1.00 17.75 1.00 19.55 1.00 20.31 1.00 19.55 1.00 17.13 1.00 19.55 1.00 19.07 1.00 20.59 1.00 21.43 1.00 21.43 1.00 20.49 1.00 20.49 1.00 20.49 1.00 20.49 1.00 20.49 1.00 20.49 1.00 20.49 1.00 20.49 1.00 20.49 1.00 20.57 1.00 19.37 1.00 19.37 1.00 19.37 1.00 16.11 1.00 18.47 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10859 10860 10861 10863 10864 10865 10866 10867 10871 10872 10873 10874 10875 10876 10877 | C O N CA CB CCJ CCJ CCJ CCJ CCJ CCJ CCJ CCJ CCJ | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 38.668 37.751 - 38.668 37.751 - 37.106 36.316 36.200 38.817 - 37.821 - 40.284 - 40.284 - 41.798 - | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.557 -6.345 -5.5771 -9.619 -9.746 10.146 10.886 10.622 -9.238 -9.117 -9.039 12.395 13.094 12.899 14.334 14.645 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.620 8.338 10.833 11.067 11.238 11.034 11.174 11.309 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 19.55 1.00 19.55 1.00 19.55 1.00 19.71 1.00 20.59 1.00 20.49 1.00 21.43 1.00 20.49 1.00 20.49 1.00 20.49 1.00 20.49 1.00 21.93 1.00 22.24 1.00 23.75 1.00 18.75 1.00 18.75 1.00 18.75 1.00 18.75 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10860 10861 10862 10863 10864 10865 10866 10867 10872 10873 10874 10875 10876 | C O N CA CB CG CD1 CCA CB CG CD1 CCA CB CG CD1 CCB CCG CD1 CCB CCB CCB CCB CCB CCB CCB CCB CCB CC | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - 37.106 36.316 36.200 38.817 - 37.821 - 40.047 - 40.284 - 41.798 - 42.007 - | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.345 -5.557 -6.345 -5.771 -9.619 -9.746 10.144 10.886 10.622 -9.238 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.696 9.620 8.338 10.833 11.067 11.238 11.034 11.174 11.309 11.660 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 19.55 1.00 17.13 1.00 19.07 1.00 20.59 1.00 20.59 1.00 20.59 1.00 21.43 1.00 20.49 1.00 20.49 1.00 21.43 1.00 20.49 1.00 21.93 1.00 21.93 1.00 22.24 1.00 23.75 1.00 18.75 1.00 18.75 1.00 18.75 1.00 18.75 1.00 18.75 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10859 10860 10861 10863 10864 10865 10866 10867 10871 10872 10873 10874 10875 10876 10877 | C O N CA CB CCJ CCJ CCJ CCJ CCJ CCJ CCJ CCJ CCJ | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - 37.106 36.316 36.316 36.200 38.817 - 37.821 - 40.284 - 40.284 - 41.798 - 42.007 - 42.505 - | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.345 -5.557 -6.345 -5.577 -9.619 -9.746 10.886 10.622 -9.238 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.620 8.338 10.833 11.067 11.238 11.034 11.174 11.309 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 19.55 1.00 19.55 1.00 19.55 1.00 19.71 1.00 20.59 1.00 20.49 1.00 21.43 1.00 20.49 1.00 20.49 1.00 20.49 1.00 20.49 1.00 21.93 1.00 22.24 1.00 23.75 1.00 18.75 1.00 18.75 1.00 18.75 1.00 18.75 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10860 10861 10862 10863 10864 10865 10866 10867 10872 10873 10874 10875 10876 | C O N CA CB CG CD1 CD2 C O N CA CB CG CD1 CD2 C C C C C C C C C C C C C C C C C C | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - 37.106 36.316 36.200 38.817 - 37.821 - 40.047 - 40.284 - 41.798 - 42.007 - | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.345 -5.557 -6.345 -5.577 -9.619 -9.746 10.886 10.622 -9.238 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.696 9.620 8.338 10.833 11.067 11.238 11.034 11.174 11.309 11.660 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 19.55 1.00 17.13 1.00 19.07 1.00 20.59 1.00 20.59 1.00 20.59 1.00 21.43 1.00 20.49 1.00 20.49 1.00 21.43 1.00 20.49 1.00 21.93 1.00 21.93 1.00 22.24 1.00 23.75 1.00 18.75 1.00 18.75 1.00 18.75 1.00 18.75 1.00 18.75 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10859 10860 10861 10862 10863 10864 10865 10866 10867 10872 10873 10874 10875 10876 10877 10878 10878 | C O N CA CB CG CD1 CD2 C O N CA CB CG CD1 CD2 C C C C C C C C C C C C C C C C C C | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 37.751 - 37.106 36.316 36.316 36.316 36.316 36.316 36.316 36.316 36.316 37.751 - 37.106 36.316 36.316 36.316 36.316 36.316 36.316 36.316 37.751 - 37.106 36.316 36.316 36.316 36.316 36.316 36.316 36.316 36.316 36.316 36.316 36.316 36.316 36.316 36.316 36.316 36.316 37.751 - 37.106 36.316 36.316 36.316 36.316 36.316 36.316 | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.345 -5.557 -6.345 -5.771 -9.619 -9.746 10.886 10.622 -9.238 -9.117 -9.039 12.395 13.094 12.899 14.334 14.972 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.696 9.620 8.338 11.067 11.238 11.174 11.309 11.660 10.003 12.349 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 20.46 1.00 19.95 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 19.55 1.00 19.67 1.00 20.59 1.00 20.59 1.00 21.43 1.00 20.49 1.00 20.97 1.00 20.97 1.00 21.93 1.00 22.24 1.00 23.75 1.00 19.39 1.00 18.75 1.00 18.75 1.00 18.75 1.00 18.75 1.00 18.75 1.00 18.75 1.00 18.75 1.00 20.87 1.00 20.87 1.00 20.87 1.00 20.87 1.00 20.87 1.00 20.87 1.00 20.87 1.00 20.87 1.00 20.87 1.00 20.87 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10857 10858 10859 10860 10861 10862 10863 10864 10865 10866 10870 10871 10872 10873 10874 10875 10876 10877 10878 10879 10879 10880 10881 10882 | C O N CA CB CC2 C C C C C C C C C C C C C C C C | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - 37.106 36.316 36.200 38.817 - 37.821 - 40.047 - 40.284 - 41.798 - 42.007 - 42.505 - 39.553 - 38.847 - | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.557 -6.345 -5.557 -6.345 -9.746 10.886 10.622 -9.238 -9.117 -9.039 12.395 13.094 12.899 14.334 14.645 16.107 14.972 15.965 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.833 10.833 11.067 11.238 11.034 11.174 11.309 11.660 10.003 12.349 12.173 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 20.46 1.00 20.46 1.00 19.95 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 19.07 1.00 18.71 1.00 19.07 1.00 20.59 1.00 21.43 1.00 20.49 1.00 20.49 1.00 21.43 1.00 20.49 1.00 21.43 1.00 23.75 1.00 18.47 1.00 19.37 1.00 18.37 1.00 18.37 1.00 22.24 1.00 23.75 1.00 18.47 1.00 20.23 1.00 20.23 1.00 20.298 1.00 18.83 1.00 18.83 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10857 10858 10859 10860 10861 10863 10864 10865 10866 10867 10872 10872 10873 10874 10875 10876 10877 10878 10879 10878 10879 10880 10880 10881 10882 10883 | C O N CA CB CG CD1 CCA CB CG CD1 CCA CB CG CD1 CCA CB CG CD1 CCA CB CC O N CCA CB CC O N CCA CB CCB CC O N CCA CB CCB CCB CCB CCB CCB CCB CCB CCB | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - 37.106 36.316 36.200 38.817 - 37.821 - 40.047 - 40.284 - 41.798 - 42.007 - 42.505 - 39.553 - 38.847 - 39.731 - | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.348 -5.855 -5.557 -6.345 -5.771 -9.619 -9.746 10.886 10.622 -9.238 -9.117 -9.039 12.395 13.094 12.899 14.334 14.645 16.107 14.972 15.965 14.411 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.620 8.338 10.833 11.067 11.238 10.34 11.174 11.309 11.660 10.003 12.349 12.173 13.543 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.95 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 19.55 1.00 19.55 1.00 19.07 1.00 20.59 1.00 20.59 1.00 20.49 1.00 20.49 1.00 20.97 1.00 20.97 1.00 20.97 1.00 23.75 1.00 16.15 1.00 18.75 1.00 18.75 1.00 18.75 1.00 20.87 1.00 20.87 1.00 20.87 1.00 20.88 1.00 20.88 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10856 10857 10858 10860 10861 10862 10863 10864 10865 10866 10867 10872 10873 10874 10875 10876 10877 10878 10879 10880 10881 10883 10883 | C O N CA CB CG CD1 CCA CB CG CD1 CCA CB CCD1 CCA CB CCD1 CCA CCB CCD1 CCA CCB CCB CCB CCB CCB CCB CCB CCB CCB | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - 37.106 36.316 36.200 38.817 - 37.821 - 40.047 - 41.798 - 42.007 - 42.505 - 39.553 - 38.847 - 39.553 - 38.847 - 39.731 - 39.088 - | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.345 -5.557 -6.345 -5.557 -6.345 -9.746 10.144 10.886 10.622 -9.238 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.696 9.696 9.696 9.338 10.833 11.067 11.238 11.349 11.374 11.309 11.660 10.003 12.349 12.173 13.543 14.741 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.68 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 19.55 1.00 17.13 1.00 19.55 1.00 19.07 1.00 20.59 1.00 20.59 1.00 20.49 1.00 20.49 1.00 20.49 1.00 20.49 1.00 20.49 1.00 20.49 1.00 21.43 1.00 20.49 1.00 21.43 1.00 20.49 1.00 21.43 1.00 20.49 1.00 21.43 1.00 20.49 1.00 21.43 1.00 20.49 1.00 20.87 1.00 18.47 1.00 18.75 1.00 18.47 1.00 20.23 1.00 20.87 1.00 18.83 1.00 18.83 1.00 18.85 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 10852 10853 10854 10855 10857 10858 10859 10860 10861 10863 10864 10865 10866 10867 10872 10872 10873 10874 10875 10876 10877 10878 10879 10878 10879 10880 10880 10881 10882 10883 | C O N CA CB CG CD1 CCA CB CG CD1 CCA CB CCD1 CCA CB CCD1 CCA CCB CCD1 CCA CCB CCB CCB CCB CCB CCB CCB CCB CCB | GLU GLU TRP | 1617 1617 1618 1618 1618 1618 1618 1618 | 42.718 - 42.527 - 42.404 41.830 41.607 40.461 39.152 38.392 38.544 40.446 39.205 37.054 37.214 36.482 40.544 40.136 39.917 - 38.668 - 37.751 - 37.106 36.316 36.200 38.817 - 37.821 - 40.047 - 40.284 - 41.798 - 42.007 - 42.505 - 39.553 - 38.847 - 39.731 - | -10.294 -11.289 -9.069 -8.855 -7.364 -6.766 -6.510 -5.939 -6.723 -6.345 -5.557 -6.345 -5.557 -6.345 -9.746 10.144 10.886 10.622 -9.238 | 9.015 9.800 10.499 10.202 11.518 11.776 11.040 11.563 10.521 12.809 9.745 9.423 10.690 12.977 11.915 11.787 12.938 10.737 10.893 9.620 8.338 10.633 11.067 11.238 10.334 11.174 11.309 11.174 11.309 11.660 10.003 12.349 12.173 13.543 | 1.00 39.51 1.00 23.15 1.00 24.44 1.00 22.84 1.00 21.59 1.00 19.95 1.00 17.75 1.00 18.42 1.00 20.31 1.00 19.55 1.00 17.13 1.00 19.55 1.00 19.55 1.00 19.07 1.00 20.59 1.00 20.59 1.00 20.49 1.00 20.49 1.00 20.97 1.00 20.97 1.00 20.97 1.00 23.75 1.00 16.15 1.00 18.75 1.00 18.75 1.00 18.75 1.00 20.87 1.00 20.87 1.00 20.87 1.00 20.88 1.00 20.88 | |

| ATOM | 10886 | CG | GLU | 1621 | 38.815 -14.561 | 17.256 | 1.00 22.60 |
|------|-------|-----|-----|------|----------------|--------|------------|
| ATOM | 10887 | CD | GLU | 1621 | 39.265 -13.760 | 18.471 | 1.00 25.26 |
| | | | | | | | |
| MOTA | 10888 | | GLU | 1621 | 39.153 -12.515 | 18.453 | 1.00 24.17 |
| MOTA | 10889 | OE2 | GLU | 1621 | 39.730 -14.383 | 19.446 | 1.00 28.44 |
| ATOM | 10890 | С | GLU | 1621 | 37.571 -14.962 | 14.599 | 1.00 16.87 |
| ATOM | 10891 | Ō | GLU | 1621 | 36.915 -15.951 | 14.909 | 1.00 16.16 |
| | | | | | | | |
| MOTA | 10892 | N | THR | 1622 | 37.023 -13.855 | 14.118 | 1.00 17.23 |
| ATOM | 10893 | CA | THR | 1622 | 35.583 -13.729 | 13.938 | 1.00 15.12 |
| ATOM | 10894 | CB | THR | 1622 | 35.238 -12.319 | 13.420 | 1.00 16.38 |
| ATOM | 10895 | OG1 | | 1622 | 35.730 -11.345 | 14.356 | 1.00 17.00 |
| | | | | | | | |
| MOTA | 10896 | CG2 | THR | 1622 | 33.727 -12.140 | 13.272 | 1.00 14.48 |
| MOTA | 10897 | С | THR | 1622 | 35.048 -14.797 | 12.985 | 1.00 15.13 |
| ATOM | 10898 | 0 | THR | 1622 | 34.064 -15.464 | 13.293 | 1.00 13.37 |
| ATOM | 10899 | N | VAL | 1623 | 35.696 -14.963 | 11.832 | 1.00 13.92 |
| | | | | | | | |
| MOTA | 10900 | CA | VAL | 1623 | 35.258 -15.969 | 10.862 | 1.00 14.72 |
| MOTA | 10901 | CB | VAL | 1623 | 36.102 -15.907 | 9.569 | 1.00 14.99 |
| MOTA | 10902 | CG1 | VAL | 1623 | 35.676 -17.017 | 8.602 | 1.00 16.56 |
| ATOM | 10903 | CG2 | VAL | 1623 | 35.936 -14.548 | 8.921 | 1.00 14.47 |
| ATOM | 10904 | C | VAL | 1623 | 35.345 -17.382 | 11.452 | 1.00 15.17 |
| | | | | | | | |
| MOTA | 10905 | 0 | VAL | 1623 | 34.424 ~18.186 | 11.308 | 1.00 13.99 |
| MOTA | 10906 | N | GLN | 1624 | 36.456 -17.680 | 12.118 | 1.00 14.83 |
| MOTA | 10907 | CA | GLN | 1624 | 36.641 -18.992 | 12.729 | 1.00 17.43 |
| ATOM | 10908 | CB | GLN | 1624 | 38.012 -19.073 | 13.415 | 1.00 20.41 |
| | | | | | | | |
| ATOM | 10909 | CG | GLN | 1624 | 39.205 -18.806 | 12.499 | 1.00 28.20 |
| MOTA | 10910 | CD | GLN | 1624 | 40.540 -18.963 | 13.210 | 1.00 31.26 |
| MOTA | 10911 | OE1 | GLN | 1624 | 40.789 -18.329 | 14.238 | 1.00 33.11 |
| ATOM | 10912 | NE2 | GLN | 1624 | 41.408 -19.809 | 12.661 | 1.00 32.88 |
| ATOM | 10913 | C | GLN | 1624 | 35.544 -19.296 | 13.755 | 1.00 15.38 |
| | | | | | | | |
| MOTA | 10914 | 0 | GLN | 1624 | 34.966 -20.384 | 13.757 | 1.00 15.85 |
| ATOM | 10915 | N | MET | 1625 | 35.266 -18.334 | 14.632 | 1.00 16.26 |
| ATOM | 10916 | CA | MET | 1625 | 34.249 -18.528 | 15.664 | 1.00 14.73 |
| ATOM | 10917 | СВ | MET | 1625 | 34.398 -17.466 | 16.758 | 1.00 15.61 |
| | | | | | | | |
| MOTA | 10918 | CG | MET | 1625 | 35.637 -17.671 | 17.623 | 1.00 18.12 |
| MOTA | 10919 | SD | MET | 1625 | 35.862 -16.357 | 18.837 | 1.00 20.56 |
| ATOM | 10920 | CE | MET | 1625 | 34.733 -16.876 | 20.128 | 1.00 24.48 |
| ATOM | 10921 | С | MET | 1625 | 32.832 -18.534 | 15.104 | 1.00 15.23 |
| | | | | | | | |
| ATOM | 10922 | 0 | MET | 1625 | 31.976 -19.288 | 15.571 | 1.00 15.05 |
| MOTA | 10923 | N | LEU | 1626 | 32.572 -17.702 | 14.101 | 1.00 16.96 |
| MOTA | 10924 | CA | LEU | 1626 | 31.240 -17.694 | 13.504 | 1.00 15.20 |
| MOTA | 10925 | CB | LEU | 1626 | 31.139 -16.617 | 12.416 | 1.00 15.28 |
| ATOM | 10926 | CG | LEU | 1626 | 30.816 -15.209 | 12.916 | 1.00 12.23 |
| | | | | | | | |
| ATOM | 10927 | | LEU | 1626 | 30.993 -14.196 | 11.790 | 1.00 12.86 |
| MOTA | 10928 | CD2 | LEU | 1626 | 29.398 -15.188 | 13.455 | 1.00 11.50 |
| MOTA | 10929 | С | LEU | 1626 | 30.947 -19.065 | 12.900 | 1.00 16.67 |
| ATOM | 10930 | 0 | LEU | 1626 | 29.905 -19.679 | 13.161 | 1.00 16.01 |
| | | | | 1627 | | | |
| MOTA | 10931 | N | THR | | 31.887 -19.548 | 12.098 | 1.00 16.42 |
| MOTA | 10932 | CA | THR | 1627 | 31.743 -20.833 | 11.423 | 1.00 19.44 |
| ATOM | 10933 | CB | THR | 1627 | 33.000 -21.152 | 10.592 | 1.00 20.87 |
| ATOM | 10934 | OG1 | THR | 1627 | 33.259 -20.061 | 9.698 | 1.00 22.73 |
| ATOM | 10935 | CG2 | THR | 1627 | 32.790 -22.424 | 9.770 | 1.00 26.46 |
| ATOM | 10936 | | THR | | 31.481 -21.983 | 12.382 | 1.00 18.98 |
| | | С | | 1627 | | | |
| MOTA | 10937 | 0 | THR | 1627 | 30.573 -22.782 | 12.168 | 1.00 20.35 |
| ATOM | 10938 | N | GLU | 1628 | 32.267 -22.072 | 13.446 | 1.00 20.15 |
| ATOM | 10939 | CA | GLU | 1628 | 32.053 -23.160 | 14.378 | 1.00 21.96 |
| MOTA | 10940 | СВ | GLU | 1628 | 33.257 -23.296 | 15.313 | 1.00 25.32 |
| ATOM | 10941 | CG | GLU | 1628 | 33.231 -22.418 | 16.525 | 1.00 28:20 |
| | | | | | | | |
| MOTA | 10942 | CD | GLU | 1628 | 34.458 -22.615 | 17.394 | 1.00 27.97 |
| MOTA | 10943 | OE1 | GLU | 1628 | 34.989 -23.748 | 17.440 | 1.00 27.80 |
| MOTA | 10944 | OE2 | GLU | 1628 | 34.884 -21.638 | 18.039 | 1.00 28.14 |
| ATOM | 10945 | C | GLU | 1628 | 30.737 -22.990 | 15.155 | 1.00 21.32 |
| | | | | | | | |
| MOTA | 10946 | 0 | GLU | 1628 | | 15.807 | 1.00 21.40 |
| MOTA | 10947 | N | ARG | 1629 | 30.127 -21.806 | 15.073 | 1.00 18.90 |
| ATOM | 10948 | CA | ARG | 1629 | 28.850 -21.555 | 15.739 | 1.00 18.94 |
| ATOM | 10949 | CB | ARG | 1629 | 28.877 -20.193 | 16.455 | 1.00 19.15 |
| ATOM | 10950 | CG | ARG | 1629 | 29.636 -20.242 | 17.778 | 1.00 15.15 |
| | | | | | | | |
| MOTA | 10951 | CD | ARG | 1629 | 30.159 -18.882 | 18.246 | 1.00 12.70 |
| ATOM | 10952 | NE | ARG | 1629 | 30.954 -19.047 | 19.460 | 1.00 13.17 |
| MOTA | 10953 | CZ | ARG | 1629 | 32.154 -19.616 | 19.498 | 1.00 12.49 |
| MOTA | 10954 | | ARG | 1629 | 32.719 -20.068 | 18.382 | 1.00 14.22 |
| MOTA | 10955 | | | | 32.778 -19.774 | 20.658 | 1.00 15.37 |
| | | NH2 | ARG | 1629 | | | |
| MOTA | 10956 | С | ARG | 1629 | 27.659 -21.633 | 14.768 | 1.00 19.42 |
| ATOM | 10957 | 0 | ARG | 1629 | 26.610 -21.029 | 15.006 | 1.00 21.03 |
| ATOM | 10958 | N | ALA | 1630 | 27.838 -22.373 | 13.671 | 1.00 19.16 |
| ATOM | 10959 | CA | ALA | 1630 | 26.792 -22.591 | 12.663 | 1.00 17.42 |
| ATOM | | | | | 25.493 -23.018 | 13.346 | 1.00 17.42 |
| | 10960 | CB | ALA | 1630 | | | |
| ATOM | 10961 | С | ALA | 1630 | 26.503 -21.444 | 11.698 | 1.00 16.92 |
| ATOM | 10962 | 0 | ALA | 1630 | 25.460 -21.433 | 11.052 | 1.00 15.55 |
| | | | | | | | |

| ATOM | 10963 | N | VAL | 1631 | 27.412 | -20.484 | 11.590 | 1.00 16.60 |
|--------------|----------------|---------|------------|--------------|------------------|-----------------|-----------------|--------------------------|
| ATOM | 10964 | CA | VAL | 1631 | 27.194 | -19.369 | 10.685 | 1.00 15.88 |
| ATOM | 10965 | CB | VAL | 1631 | 27.282 | -18.019 | 11.436 | 1.00 17.04 |
| ATOM | 10966 | CG1 | VAL | 1631 | 26.996 | -16.863 | 10.477 | 1.00 15.90 |
| ATOM | 10967 | CG2 | VAL | 1631 | 26.280 | -17.994 | 12.590 | 1.00 18.38 |
| ATOM | 10968 | Ċ | VAL | 1631 | 28.200 | -19.357 | 9.534 | 1.00 15.71 |
| ATOM | 10969 | Ō | VAL | 1631 | | -19.046 | 9.728 | 1.00 17.57 |
| ATOM | 10970 | N | PRO | 1632 | 27.760 | | 8.318 | 1.00 16.10 |
| ATOM | 10971 | CD | PRO | 1632 | | -20.292 | 7.901 | 1.00 14.50 |
| ATOM | 10972 | CA | PRO | 1632 | | -19.706 | 7.200 | 1.00 15.24 |
| ATOM | 10973 | CB | PRO | 1632 | 27.961 | | 6.083 | 1.00 15.98 |
| ATOM | 10974 | CG | PRO | 1632 | 26.552 | -20.188 | 6.393 | 1.00 20.78 |
| ATOM | 10975 | С | PRO | 1632 | 29.025 | -18.255 | 6.857 | 1.00 16.57 |
| ATOM | 10976 | 0 | PRO | 1632 | 28.156 | | 6.933 | 1.00 15.01 |
| ATOM | 10977 | N | VAL | 1633 | 30.269 | -18.003 | 6.478 | 1.00 14.68 |
| ATOM | 10978 | CA | VAL | 1633 | 30.703 | -16.654 | 6.174 | 1.00 14.60 |
| ATOM | 10979 | CB | VAL | 1633 | 31.808 | -16.213 | 7.157 | 1.00 16.39 |
| ATOM | 10980 | CG1 | VAL | 1633 | 32.210 | -14.773 | 6.874 | 1.00 16.35 |
| ATOM | 10981 | | VAL | 1633 | 31.320 | -16.371 | 8.593 | 1.00 15.41 |
| MOTA | 10982 | С | VAL | 1633 | 31.237 | -16.462 | 4.770 | 1.00 14.92 |
| ATOM | 10983 | 0 | VAL | 1633 | 31.952 | -17.311 | 4.234 | 1.00 14.86 |
| ATOM | 10984 | N | CYS | 1634 | 30.875 | -15.332 | 4.180 | 1.00 13.16 |
| ATOM | 10985 | CA | CYS | 1634 | 31.352 | -14.972 | 2.855 | 1.00 15.22 |
| ATOM | 10986 | CB. | CYS | 1634 | 30.186 | -14.545 | 1.955 | 1.00 14.14 |
| MOTA | 10987 | SG | CYS | 1634 | 30.713 | -13.922 | 0.336 | 1.00 17.65 |
| ATOM | 10988 | С | CYS | 1634 | 32.277 | -13.794 | 3.132 | 1.00 14.44 |
| MOTA | 10989 | 0 | CYS | 1634 | 31.929 | -12.892 | 3.887 | 1.00 15.27 |
| MOTA | 10990 | Ń | GLY | 1635 | 33.471 | -13.816 | 2.558 | 1.00 15.52 |
| MOTA | 10991 | CA | GLY | 1635 | 34.400 | -12.723 | 2.779 | 1.00 14.14 |
| MOTA | 10992 | С | GLY | 1635 | 34.162 | -11.615 | 1.771 | 1.00 15.47 |
| MOTA | 10993 | 0 | GLY | 1635 | 33.352 | -11.776 | 0.866 | 1.00 16.16 |
| MOTA | 10994 | N | HIS | 1636 | 34.867 | -10.498 | 1.918 | 1.00 16.26 |
| MOTA | 10995 | CA | HIS | 1636 | 34.709 | -9.364 | 1.009 | 1.00 18.95 |
| MOTA | 10996 | CB | HIS | 1636 | 33.468 | -8.553 | 1.413 | 1.00 19.60 |
| ATOM | 10997 | CG | HIS | 1636 | 33.099 | -7.460 | 0.456 | 1.00 20.41 |
| ATOM | 10998 | CD2 | HIS | 1636 | 33.752 | -6.934 | -0.607 | 1.00 20.13 |
| ATOM | 10999 | ND1 | HIS | 1636 | 31.917 | -6.757 | 0.561 | 1.00 20.81 |
| ATOM | 11000 | CE1 | HIS | 1636 | 31.858 | -5.847 | -0.393 | 1.00 20.55 |
| MOTA | 11001 | NE2 | HIS | 1636 | 32.960 | -5.933 | -1.116 | 1.00 20.46 |
| MOTA | 11002 | С | HIS | 1636 | 35.959 | -8.491 | 1.073 | 1.00 21.06 |
| ATOM | 11003 | 0 | HIS | 1636 | 36.171 | -7.769 | 2.050 | 1.00 23.03 |
| MOTA | 11004 | N | LEU | 1637 | 36.783 | -8.571 | 0.030 | 1.00 22.97 |
| MOTA | 11005 | CA | LEU | 1637 | 38.028 | -7.804 | -0.050 | 1.00 24.89 |
| ATOM . | 11006 | CB | LEU | 1637 | 39.227 | -8.755 | -0.153 | 1.00 24.90 |
| ATOM | 11007 | CG- | LEU | 1637 | 39.479 | -9.659 | 1.057 | 1.00 26.13 |
| MOTA | 11008 | | LEU | 1637 | 40.618 | -10.621 | 0.773 | 1.00 24.93 |
| MOTA | 11009 | | LEU | 1637 | 39.804 | -8.798 | 2.267 | 1.00 26.07 |
| MOTA | 11010 | С | LEU | 1637 | 38.026 | -6.854 | -1.243 | 1.00 26.65 |
| ATOM | 11011 | 0 | LEU | 1637 | 37.199 | -6.978 | -2.147 | 1.00 24.18 |
| ATOM | 11012 | N | GLY | 1638 | 38.962 | -5.909 | -1.234 | 1.00 28.25 |
| MOTA | 11013 | CA | GLY | 1638 | 39.063 | -4.941 | -2.309 | 1.00 28.56 |
| MOTA | 11014 | С | GLY | | 38.402 | -3.634 | | 1.00 29.01 |
| MOTA | 11015 | 0 | GLY | 1638 | 38.664 | -3.081 | -0.858 | 1.00 29.30 |
| MOTA | 11016 | N | LEU | 1639 | 37.537 | | -2.805 | 1.00 28.17 |
| ATOM | 11017 | CA | LEU | 1639 | 36.824 | -1.898 | -2.566 | 1.00 27.72 |
| MOTA | 11018 | CB | LEU | 1639 | 36.311 | -1.348 | -3.899 | 1.00 29.18 |
| ATOM | 11019 | CG | LEU | 1639 | 36.026 | 0.153 | -3.987 | 1.00 30.77 |
| ATOM | 11020 | | LEU | 1639 | 35.697 | 0.527 | -5.427 | 1.00 31.76 |
| ATOM | 11021 | | LEU | 1639 | 34.890 | 0.522 | -3.066 | 1.00 30.98 |
| ATOM | 11022 | С | LEU | 1639 | 35.657 | -2.190 | -1.620 | 1.00 28.43 |
| MOTA | 11023 | 0 | LEU | 1639 | 34.575 | -2.581 | -2.063 | 1.00 26.50 |
| MOTA | 11024 | N | THR | 1640 | 35.890 | -2.013 | -0.320 | 1.00 28.20 |
| MOTA | 11025 | CA | THR | 1640 | 34.866 | -2.259 | 0.698 | 1.00 28.91 |
| ATOM | 11026 | CB | THR | 1640 | 35.482 | -2.866 | 1.970 | 1.00 29.17 |
| ATOM | 11027 | OG1 | | 1640 | 36.517 | -2.006 | 2.462 | 1.00 30.62 |
| MOTA | 11028 | CG2 | | 1640 | 36.068 | -4.236 | 1.670 1.057 | 1.00 30.17 1.00 28.17 |
| MOTA | 11029 | С | THR | 1640 | 34.171 | -0.951 | | |
| MOTA | 11030 | 0 | THR | 1640 | 34.667 | -0.177 | 1.874 | 1.00 29.15 |
| MOTA | 11031 | N CD | PRO | 1641 | | -0.706 | 0.463 | 1.00 27.49 |
| ATOM | 11032 | CD | PRO | 1641 | 32.251 | -1.695 | -0.339 | 1.00 27.96 1.00 26.18 |
| ATOM | 11033 | CA | PRO | 1641 | 32.189 | 0.502 | 0.674 -0.092 | 1.00 26.18 |
| ATOM | 11034 | CB. | PRO | 1641 | 30.897 | 0.202 -1.290 | -0.092 | 1.00 20.35 |
| ATOM | 11035 | CG | PRO | 1641 | 30.832 | 0.977 | 2.104 | 1.00 25.02 |
| MOTA | 11036 | С | PRO | 1641 | 31.952 | 2.174 | 2.104 | 1.00 25.02 |
| MOTA MOTA | 11037 11038 | O N | PRO | 1641 1642 | 31.763 31.968 | 0.064 | 3.070 | 1.00 24.04 |
| ATOM | 11038 | N CA | GLN GLN | 1642 | 31.768 | 0.475 | 4.459 | 1.00 23.18 |
| AIUM | 11033 | CM | GIII | TOAZ | 21.708 | 0.4/3 | 4.400 | 2.00 23.00 |

| ATOM | 11040 | СВ | GLN | 1642 | 31.661 | -0.751 | 5.369 | 1.00 24.34 |
|-------|-------|-----|-----|------|--------|--------|------------------|------------|
| MOTA | 11041 | CG | GLN | 1642 | 30.249 | -1.307 | 5.471 | 1.00 22.71 |
| ATOM | 11042 | CD | GLN | 1642 | 30.192 | -2.633 | 6.204 | 1.00 25.04 |
| ATOM | 11042 | OE1 | | 1642 | 31.017 | -2.910 | 7.075 | 1.00 23.03 |
| | | NE2 | | 1642 | 29.204 | -3.456 | 5.865 | 1.00 23.05 |
| ATOM | 11044 | | | | | | 4.911 | 1.00 24.23 |
| MOTA | 11045 | С | GLN | 1642 | 32.922 | 1.367 | | |
| MOTA | 11046 | 0 | GLN | 1642 | 32.781 | 2.160 | 5.842 | 1.00 24.32 |
| MOTA | 11047 | N | SER | 1643 | 34.061 | 1.235 | 4.237 | 1.00 23.66 |
| MOTA | 11048 | CA | SER | 1643 | 35.246 | 2.028 | 4.559 | 1.00 24.17 |
| MOTA | 11049 | CB | SER | 1643 | 36.478 | 1.126 | 4.596 | 1.00 23.24 |
| ATOM | 11050 | OG | SER | 1643 | 36.342 | 0.116 | 5.570 | 1.00 21.44 |
| MOTA | 11051 | С | SER | 1643 | 35.474 | 3.157 | 3.556 | 1.00 25.48 |
| MOTA | 11052 | 0 | SER | 1643 | 36.602 | 3.618 | 3.368 | 1.00 24.46 |
| ATOM | 11053 | N | VAL | 1644 | 34.400 | 3.598 | 2.908 | 1.00 26.06 |
| ATOM | 11054 | CA | VAL | 1644 | 34.502 | 4.671 | 1.924 | 1.00 26.14 |
| ATOM | 11055 | CB | VAL | 1644 | 33.109 | 5.080 | 1.402 | 1.00 25.49 |
| MOTA | 11056 | CG1 | VAL | 1644 | 32.258 | 5.623 | 2.541 | 1.00 26.03 |
| MOTA | 11057 | CG2 | | 1644 | 33.250 | 6.110 | 0.293 | 1.00 25.29 |
| ATOM | 11058 | С | VAL | 1644 | 35.209 | 5.905 | 2.501 | 1.00 27.56 |
| MOTA | 11059 | Ö | VAL | 1644 | 36.063 | 6.500 | 1.842 | 1.00 27.45 |
| MOTA | 11060 | N | ASN | 1645 | 34.866 | 6.282 | 3.732 | 1.00 27.89 |
| ATOM | 11061 | CA | ASN | 1645 | 35.480 | 7.452 | 4.359 | 1.00 27.05 |
| | | | | | | | | |
| ATOM | 11062 | CB | ASN | 1645 | 34.779 | 7.776 | 5.682 | 1.00 27.21 |
| MOTA | 11063 | CG | ASN | 1645 | 33.331 | 8.190 | 5.486 | 1.00 25.74 |
| MOTA | 11064 | | ASN | 1645 | 33.045 | 9.268 | 4.967 | 1.00 22.31 |
| ATOM | 11065 | | ASN | 1645 | 32.408 | 7.321 | 5.888 | 1.00 25.99 |
| MOTA | 11066 | С | ASN | 1645 | 36.971 | 7.241 | 4.599 | 1.00 29.33 |
| MOTA | 11067 | 0 | ASN | 1645 | 37.735 | 8.205 | 4.676 | 1.00 29.64 |
| ATOM | 11068 | N | ILE | 1646 | 37.373 | 5.978 | 4.715 | 1.00 30.28 |
| MOTA | 11069 | CA | ILE | 1646 | 38.773 | 5.626 | 4.931 | 1.00 31.32 |
| ATOM | 11070 | CB | ILE | 1646 | 38.929 | 4.153 | 5.396 | 1.00 31.95 |
| MOTA | 11071 | CG2 | ILE | 1646 | 40.399 | 3.752 | 5.377 | 1.00 31.20 |
| MOTA | 11072 | CG1 | ILE | 1646 | 38.355 | 3.977 | 6.806 | 1.00 31.77 |
| ATOM | 11073 | CD1 | ILE | 1646 | 39.071 | 4.789 | 7.862 | 1.00 31.01 |
| ATOM | 11074 | С | ILE | 1646 | 39.562 | 5.809 | 3.636 | 1.00 33.51 |
| MOTA | 11075 | .0 | ILE | 1646 | 40.655 | 6.377 | 3.644 | 1.00 34.28 |
| MOTA | 11075 | N | PHE | 1647 | 39.006 | 5.324 | 2.526 | 1.00 34.25 |
| | | CA | | 1647 | 39.664 | 5.439 | 1.225 | 1.00 34.33 |
| ATOM | 11077 | | PHE | | | | | |
| ATOM | 11078 | CB | PHE | 1647 | 39.083 | 4.429 | 0.227 | 1.00 36.28 |
| MOTA | 11079 | CG | PHE | 1647 | 39.051 | 3.014 | 0.734 | 1.00 37.21 |
| MOTA | 11080 | | PHE | 1647 | 40.183 | 2.435 | 1.300 | 1.00 37.15 |
| ATOM | 11081 | CD2 | | 1647 | 37.885 | 2.257 | 0.638 | 1.00 36.77 |
| MOTA | 11082 | CE1 | | 1647 | 40.154 | 1.120 | 1.763 | 1.00 38.58 |
| MOTA | 11083 | CE2 | | 1647 | 37.845 | 0.943 | 1.096 | 1.00 36.69 |
| ATOM | 11084 | cz | PHE | 1647 | 38.981 | 0.373 | 1.661 | 1.00 38.01 |
| MOTA: | 11085 | С | PHE | 1647 | 39.512 | 6.840 | 0.643 | 1.00 36.39 |
| ATOM | 11086 | 0 | PHE | 1647 | 40.280 | 7.243 | -0.233 | 1.00 36.05 |
| ATOM | 11087 | N | GLY | 1648 | 38.518 | 7.577 | 1.130 | 1.00 36.62 |
| ATOM | 11088 | CA | GLY | 1648 | 38.279 | 8.919 | 0.630 | 1.00 38.30 |
| ATOM | 11089 | С | GLY | 1648 | 37.421 | 8.878 | -0.622 | 1.00 40.02 |
| ATOM | 11090 | 0 | GLY | 1648 | 37.406 | 9.822 | -1.413 | 1.00 40.07 |
| ATOM | 11091 | N | GLY | 1649 | 36.703 | 7.773 | -0.796 | 1.00 40.99 |
| ATOM | 11092 | CA | GLY | 1649 | 35.846 | 7.609 | -1.956 | 1.00 42.04 |
| ATOM | 11093 | C | GLY | 1649 | 35.898 | 6.184 | -2.477 | 1.00 42.47 |
| ATOM | 11093 | 0 | GLY | 1649 | 36.534 | 5.324 | -1.876 | 1.00 42.47 |
| MOTA | 11095 | N | TYR | 1650 | 35.229 | 5.927 | -3.596 | 1.00 44.57 |
| ATOM | 11095 | CA | TYR | 1650 | 35.224 | 4.592 | -4.178 | 1.00 45.61 |
| | | | | | | | | 1.00 45.61 |
| ATOM | 11097 | CB | TYR | 1650 | 33.839 | 4.258 | -4.735 | |
| ATOM | 11098 | CG | TYR | 1650 | 32.731 | 4.386 | -3.713 | 1.00 48.02 |
| ATOM | 11099 | | TYR | 1650 | 32.142 | 5.623 | -3.448 | 1.00 47.87 |
| ATOM | 11100 | | TYR | 1650 | 31.142 | 5.753 | -2.487 | 1.00 48.46 |
| MOTA | 11101 | | TYR | 1650 | 32.291 | 3.275 | -2.988 | 1.00 48.35 |
| ATOM | 11102 | CE2 | TYR | 1650 | 31.291 | 3.394 | -2.021 | 1.00 48.79 |
| MOTA | 11103 | CZ | TYR | 1650 | 30.722 | 4.637 | -1.777 | 1.00 48.77 |
| MOTA | 11104 | ОН | TYR | 1650 | 29.735 | 4.767 | -0.827 | 1.00 48.30 |
| MOTA | 11105 | С | TYR | 1650 | 36.272 | 4.498 | -5.280 | 1.00 46.09 |
| ATOM | 11106 | 0 | TYR | 1650 | 35.975 | 4.697 | -6.458 | 1.00 45.93 |
| ATOM | 11107 | N | LYS | 1651 | 37.503 | 4.195 | -4.881 | 1.00 46.34 |
| ATOM | 11108 | CA | LYS | 1651 | 38.614 | 4.077 | -5.815 | 1.00 46.77 |
| ATOM | 11109 | CB | LYS | 1651 | 39.805 | 4.890 | -5.306 | 1.00 47.81 |
| ATOM | 11110 | CG | LYS | 1651 | 39.467 | 6.325 | -4.935 | 1.00 49.04 |
| ATOM | 11111 | CD | LYS | 1651 | 40.686 | 7.053 | -4.385 | 1.00 50.24 |
| ATOM | 11111 | CE | LYS | 1651 | 40.343 | 8.473 | -3.962 | 1.00 50.24 |
| | | | | | | 9.208 | -3.468 | 1.00 51.45 |
| ATOM | 11113 | NZ | LYS | 1651 | 41.543 | | | 1.00 33.01 |
| ATOM | 11114 | C | LYS | 1651 | 39.026 | 2.618 | -5.982 -5.087 | 1.00 46.02 |
| MOTA | 11115 | 0 | LYS | 1651 | 38.815 | 1.797 | -5.087 | |
| MOTA | 11116 | N | VAL | 1652 | 39.614 | 2.300 | -7.131 | 1.00 46.03 |
| | | | | | | | | |

| ATOM | 11117 | CA | VAL | 1652 | 40.063 | 0.941 | -7.409 | 1.00 45.48 |
|------|-------|-----|-------|------|--------|---------|---------|------------|
| MOTA | 11118 | CB | VAL | 1652 | 40.715 | 0.838 | -8.803 | 1.00 45.22 |
| ATOM | 11119 | | VAL | 1652 | 41.216 | -0.577 | -9.039 | 1.00 45.09 |
| ATOM | 11120 | | VAL | 1652 | 39.708 | 1.228 | -9.874 | 1.00 44.78 |
| ATOM | 11121 | C | VAL | 1652 | 41.080 | 0.510 | -6.360 | 1.00 45.62 |
| ATOM | 11122 | ō | VAL | 1652 | 41.910 | 1.307 | -5.921 | 1.00 44.90 |
| ATOM | 11123 | N | GLN | 1653 | 41.012 | -0.755 | -5.963 | 1.00 45.29 |
| ATOM | 11124 | CA | GLN | 1653 | 41.917 | -1.286 | -4.955 | 1.00 45.81 |
| ATOM | 11125 | CB | GLN | 1653 | 41.108 | -1.795 | -3.758 | 1.00 46.31 |
| ATOM | 11126 | CG | GLN | 1653 | 41.733 | -1.510 | -2.405 | 1.00 47.72 |
| ATOM | 11127 | CD | GLN | 1653 | 41.812 | -0.025 | -2.097 | 1.00 47.56 |
| ATOM | 11128 | | GLN | 1653 | 40.805 | 0.683 | -2.129 | 1.00 47.95 |
| ATOM | 11129 | | GLN | 1653 | 43.011 | 0.451 | -1.790 | 1.00 49.46 |
| ATOM | 11130 | C | GLN | 1653 | 42.745 | -2.422 | -5.549 | 1.00 45.65 |
| ATOM | 11131 | Ö | GLN | 1653 | 42.340 | -3.046 | -6.529 | 1.00 45.37 |
| ATOM | 11132 | N | GLY | 1654 | 43.907 | -2.686 | -4.957 | 1.00 45.93 |
| ATOM | 11133 | CA | GLY | 1654 | 44.758 | -3.753 | -5.456 | 1.00 46.97 |
| MOTA | 11134 | C | GLY | 1654 | 45.912 | -3.277 | -6.324 | 1.00 47.53 |
| ATOM | 11135 | o | GLY | 1654 | 46.917 | -3.974 | -6.457 | 1.00 46.50 |
| ATOM | 11136 | N | ARG | 1655 | 45.763 | -2.096 | -6.920 | 1.00 48.61 |
| ATOM | 11137 | CA | ARG | 1655 | 46.793 | -1.511 | -7.778 | 1.00 49.79 |
| ATOM | 11137 | CB | ARG | 1655 | 46.421 | -0.067 | -8.141 | 1.00 50.69 |
| ATOM | 11139 | CG | ARG | 1655 | 45.152 | 0.090 | -8.980 | 1.00 51.67 |
| | | | | 1655 | 45.449 | | -10.469 | 1.00 52.58 |
| ATOM | 11140 | CD | ARG | | 44.245 | | -11.297 | 1.00 52.70 |
| ATOM | 11141 | NE | ARG | 1655 | | | -11.329 | 1.00 52.70 |
| ATOM | 11142 | CZ | ARG | 1655 | 43.421 | | | 1.00 52.20 |
| MOTA | 11143 | | ARG . | 1655 | 43.658 | | -10.574 | |
| MOTA | 11144 | NH2 | ARG | 1655 | 42.360 | | -12.125 | 1.00 51.43 |
| ATOM | 11145 | C | ARG | 1655 | 48.146 | -1.512 | -7.071 | 1.00 50.62 |
| MOTA | 11146 | 0 | ARG | 1655 | 48.328 | -0.826 | -6.065 | 1.00 50.32 |
| MOTA | 11147 | N | GLY | 1656 | 49.093 | -2.282 | -7.597 | 1.00 51.16 |
| MOTA | 11148 | CA | GLY | 1656 | 50.410 | -2.339 | -6.989 | 1.00 52.70 |
| MOTA | 11149 | C | GĻY | 1656 | 50.786 | -3.730 | -6.522 | 1.00 53.14 |
| MOTA | 11150 | 0 | GLY | 1656 | 49.959 | -4.640 | -6.528 | 1.00 53.30 |
| MOTA | 11151 | N | ASP | 1657 | 52.041 | -3.898 | -6.119 | 1.00 53.65 |
| MOTA | 11152 | CA | ASP | 1657 | 52.523 | -5.190 | -5.649 | 1.00 53.80 |
| MOTA | 11153 | CB | ASP | 1657 | 54.034 | -5.308 | -5.870 | 1.00 55.47 |
| MOTA | 11154 | CG | ASP | 1657 | 54.406 | -5.377 | -7.340 | 1.00 56.62 |
| MOTA | 11155 | | ASP | 1657 | 53.962 | -6.327 | -8.022 | 1.00 56.60 |
| MOTA | 11156 | OD2 | ASP | 1657 | 55.144 | -4.484 | -7.812 | 1.00 57.58 |
| ATOM | 11157 | С | ASP | 1657 | 52.204 | -5.392 | -4.173 | 1.00 53.09 |
| MOTA | 11158 | 0 | ASP | 1657 | 51.620 | -6.404 | -3.793 | 1.00 52.84 |
| MOTA | 11159 | N | GLU | 1658 | 52.586 | -4.424 | -3.347 | 1.00 52.53 |
| MOTA | 11160 | CA | GLU | 1658 | 52.340 | -4.507 | -1.912 | 1.00 52.30 |
| ATOM | 11161 | CB | GLU | 1658 | 52.820 | -3.232 | -1.214 | 1.00 53.11 |
| MOTA | 11162 | CG | GLU | 1658 | 52.733 | -3.294 | 0.306 | 1.00 54.62 |
| ATOM | 11163 | CD | GLU | 1658 | 53.180 | -2.007 | 0.973 | 1.00 55.75 |
| ATOM | 11164 | OE1 | GLU | 1658 | 54319 | -1.562 | 0.708 | 1.00 56.22 |
| MOTA | 11165 | OE2 | GLU | 1658 | 52.393 | -1.443 | 1.768 | 1.00 55.93 |
| MOTA | 11166 | С | GLU | 1658 | 50.859 | -4.722 | -1.616 | 1.00 51.14 |
| ATOM | 11167 | 0 | GLU | 1658 | 50.491 | -5.640 | -0.882 | 1.00 50.90 |
| ATOM | 11168 | N | ALA | 1659 | 50.015 | -3.870 | -2.190 | 1.00 49.84 |
| MOTA | 11169 | CA | ALA | 1659 | 48.573 | -3.969 | -1.990 | 1.00 47.95 |
| MOTA | 11170 | CB | ALA | 1659 | 47.869 | -2.804 | -2.675 | 1.00 48.45 |
| ATOM | 11171 | С | ALA | 1659 | 48.048 | -5.293 | -2.535 | 1.00 46.33 |
| ATOM | 11172 | 0 | ALA | 1659 | 47.280 | -5.987 | -1.869 | 1.00 46.58 |
| MOTA | 11173 | N | GLY | 1660 | 48.470 | -5.635 | -3.748 | 1.00 44.15 |
| ATOM | 11174 | CA | GLY | 1660 | 48.035 | -6.874 | -4.363 | 1.00 41.45 |
| ATOM | 11175 | C | GLY | 1660 | 48.372 | -8.095 | -3.529 | 1.00 40.33 |
| ATOM | 11176 | 0 | GLY | 1660 | 47.507 | -8.925 | -3.260 | 1.00 38.67 |
| ATOM | 11177 | N | ASP | 1661 | 49.630 | -8.209 | -3.114 | 1.00 39.99 |
| MOTA | 11178 | CA | ASP | 1661 | 50.055 | -9.348 | -2.312 | 1.00 39.26 |
| ATOM | 11179 | CB | ASP | 1661 | 51.563 | -9.293 | -2.058 | 1.00 42.10 |
| ATOM | 11180 | CG | ASP | 1661 | 52.368 | -9.258 | -3.340 | 1.00 42.83 |
| MOTA | 11181 | OD1 | ASP | 1661 | 52.150 | -10.129 | -4.208 | 1.00 42.87 |
| ATOM | 11182 | | ASP | 1661 | 53.223 | -8.360 | -3.477 | 1.00 45.93 |
| MOTA | 11183 | С | ASP | 1661 | 49.317 | -9.386 | -0.982 | 1.00 38.30 |
| MOTA | 11184 | 0 | ASP | 1661 | 49.029 | -10.460 | -0.455 | 1.00 36.90 |
| ATOM | 11185 | N | GLN | 1662 | 49.014 | -8.211 | -0.442 | 1.00 37.31 |
| ATOM | 11186 | CA | GLN | 1662 | 48.306 | -8.124 | 0.829 | 1.00 37.91 |
| MOTA | 11187 | CB | GLN | 1662 | 48.299 | -6.678 | 1.336 | 1.00 39.32 |
| MOTA | 11188 | CG | GLN | 1662 | 47.557 | -6.500 | 2.647 | 1.00 42.13 |
| ATOM | 11189 | CD | GLN | 1662 | 47.934 | -7.555 | 3.671 | 1.00 43.63 |
| MOTA | 11190 | | GLN | 1662 | 49.108 | -7.733 | 3.993 | 1.00 44.57 |
| ATOM | 11191 | | GLN | 1662 | 46.937 | -8.261 | 4.186 | 1.00 45.08 |
| ATOM | 11192 | С | GLN | 1662 | 46.872 | -8.631 | 0.694 | 1.00 36.59 |
| MOTA | 11193 | 0 | GLN | 1662 | 46.316 | -9.209 | 1.632 | 1.00 35.25 |
| | | | | | | | | |

| MOTA | 11194 | N | LEU | 1663 | 46.278 | -8.408 | -0.474 | 1.00 | 36.15 |
|--------|-------|-----|-------|------|--------|---------|--------|------|--------|
| ATOM | 11195 | CA | LEU | 1663 | 44.911 | -8.851 | -0.730 | | 35.64 |
| MOTA | 11196 | СВ | LEU | 1663 | 44.359 | -8.190 | -1.999 | | 37.34 |
| ATOM | 11197 | CG | LEU | 1663 | 44.061 | -6.686 | -1.919 | | 39.82 |
| | 11198 | | LEU | 1663 | 43.626 | -6.168 | -3.283 | | 40.42 |
| MOTA | | | | | | | | | |
| MOTA | 11199 | CD2 | | 1663 | 42.971 | -6.434 | -0.884 | | 40.78 |
| MOTA | 11200 | С | LEU | 1663 | | -10.367 | -0.875 | | 33.87 |
| MOTA | 11201 | 0 | LEU | 1663 | 43.997 | -11.030 | -0.333 | | 33.09 |
| MOTA | 11202 | N | LEU | 1664 | | -10.912 | -1.604 | | 31.69 |
| ATOM | 11203 | CA | LEU | 1664 | | -12.353 | -1.808 | | 30.95 |
| ATOM | 11204 | CB | LEU | 1664 | 47.102 | -12.690 | -2.736 | 1.00 | 34.05 |
| ATOM | 11205 | CG | LEU | 1664 | | -13.905 | -3.655 | 1.00 | 35.86 |
| ATOM | 11206 | CD1 | LEU | 1664 | 48.242 | -14.089 | -4.444 | 1.00 | 37.45 |
| ATOM | 11207 | | LEU | 1664 | | -15.155 | -2.853 | 1.00 | 36.48 |
| ATOM | 11208 | C | LEU | 1664 | | -13.026 | -0.454 | | 29.09 |
| ATOM | 11209 | o | LEU | 1664 | • | -14.107 | -0.190 | | 28.40 |
| | | | | | | | 0.403 | | 26.84 |
| MOTA | 11210 | N | SER | 1665 | | -12.375 | | | |
| ATOM | 11211 | CA | SER | 1665 | | -12.897 | 1.733 | | 25.84 |
| ATOM | 11212 | CB | SER | 1665 | | -12.017 | 2.447 | | 26.63 |
| ATOM | 11213 | OG | SER | 1665 | | -12.558 | 3.713 | | 28.52 |
| MOTA | 11214 | C | SER | 1665 | 45.892 | -12.931 | 2.533 | 1.00 | 24.57 |
| ATOM | 11215 | 0 | SER | 1665 | 45.552 | -13.949 | 3.132 | 1.00 | 23.68 |
| ATOM | 11216 | N | ASP | 1666 | 45.166 | -11.815 | 2.532 | 1.00 | 24.47 |
| ATOM | 11217 | CA | ASP | 1666 | 43.901 | -11.738 | 3.258 | 1.00 | 25.90 |
| ATOM | 11218 | CB | ASP | 1666 | | -10.328 | 3.170 | 1.00 | 25.16 |
| ATOM | 11219 | CG | ASP | 1666 | 44.089 | -9.296 | 3.957 | | 27.13 |
| ATOM | 11220 | | ASP | 1666 | 44.664 | -9.652 | 5.009 | | 26.45 |
| | 11221 | | ASP | 1666 | 44.130 | -8.117 | 3.534 | | 27.04 |
| ATOM | | | | | | | | | |
| MOTA | 11222 | С | ASP | 1666 | | -12.759 | 2.714 | | 25.78 |
| ATOM | 11223 | 0 | ASP | 1666 | | -13.382 | 3.473 | | 27.18 |
| MOTA | 11224 | N | ALA | 1667 | | -12.936 | 1.397 | | 25.37 |
| ATOM | 11225 | CA | ALA | 1667 | 42.013 | -13.893 | 0.765 | | 24.67 |
| ATOM | 11226 | CB | ALA | 1667 | 42.187 | -13.849 | -0.754 | 1.00 | 24.78 |
| ATOM | 11227 | C | ALA | 1667 | 42.297 | -15.294 | 1.287 | 1.00 | 24.19 |
| ATOM | 11228 | 0 | ALA | 1667 | 41.382 | -16.026 | 1.673 | 1.00 | 22.33 |
| ATOM | 11229 | N | LEU | 1668 | 43.570 | -15.673 | 1.303 | 1.00 | 23.07 |
| ATOM | 11230 | CA | LEU | 1668 | | -16.996 | 1.792 | | 22.47 |
| MOTA | 11231 | CB | LEU | 1668 | 45.434 | -17.256 | 1.506 | | 23.09 |
| ATOM | 11232 | CG | LEU | 1668 | 45.767 | -17.598 | 0.047 | | 23.46 |
| | | | | | | | | | 24.35 |
| ATOM | 11233 | | LEU | 1668 | 47.259 | -17.456 | -0.188 | | |
| MOTA | 11234 | | LEU | 1668 | | -19.006 | ÷0.278 | | 23.63 |
| MOTA | 11235 | С | LEU | 1668 | | -17.140 | 3.288 | | 22.33 |
| MOTA | 11236 | 0 | LEU | 1668 | | -18.211 | 3.751 | | 22.16 |
| MOTA | 11237 | N | ALA | 1669 | | -16.059 | 4.038 | | 22.43 |
| MOTA | 11238 | CA | ALA | 1669 | 43.633 | -16.083 | 5.479 | 1.00 | 22.18 |
| ATOM · | 11239 | CB | ALA | 1669 | 44.086 | -14.782 | 6.111 | 1.00 | 23.50 |
| ATOM | 11240 | С | ALA | 1669 | 42.153 | -16.328 | 5.775 | 1.00 | 21.87 |
| ATOM | 11241 | 0 | ALA | 1669 | 41.809 | -17.177 | 6.600 | 1.00 | 22.22 |
| ATOM | 11242 | N | LEU | 1670 | | -15.585 | 5.098 | | 20.26 |
| ATOM | 11243 | CA | LEU | 1670 | | -15.730 | 5.288 | 1.00 | 18.56 |
| ATOM | 11244 | CB | LEU | 1670 | | -14.737 | 4.401 | | 19.24 |
| | 11244 | CG | LEU | 1670 | | -13.260 | 4.755 | | 18.45 |
| ATOM | | | | | | | | | |
| MOTA | 11246 | | LEU | 1670 | | -12.375 | 3.662 | | 19.75 |
| MOTA | 11247 | | LEU | 1670 | | -12.973 | 6.086 | | 19.43 |
| MOTA | 11248 | С | LEU | 1670 | | -17.146 | 4.962 | | 19.70 |
| MOTA | 11249 | 0 | LEU | 1670 | 38.571 | -17.714 | 5.659 | | 18.51 |
| MOTA | 11250 | N | GLU | 1671 | 39.963 | -17.720 | 3.901 | 1.00 | 18.99 |
| MOTA | 11251 | CA | GLU | 1671 | 39.603 | -19.079 | 3.518 | 1.00 | 19.04 |
| MOTA | 11252 | CB | GLU | 1671 | 40.303 | -19.474 | 2.215 | 1.00 | 19.59 |
| MOTA | 11253 | CG | GLU | 1671 | 40.072 | -20.929 | 1.816 | 1.00 | 22.01 |
| MOTA | 11254 | CD | GLU | 1671 | 40.790 | -21.305 | 0.530 | 1:00 | 24.31 |
| ATOM | 11255 | | GLU | 1671 | | -21.096 | 0.458 | | 23'.91 |
| ATOM | 11256 | | GLU | 1671 | 40.128 | -21.804 | -0.398 | | 27.07 |
| ATOM | 11257 | C | GLU | 1671 | 39.978 | -20.070 | 4.616 | | 18.25 |
| | | | | 1671 | | | | | 17.58 |
| MOTA | 11258 | 0 | GLU | | | -20.901 | 5.016 | | |
| ATOM | 11259 | N | ALA | 1672 | | -19.985 | 5.095 | | 19.38 |
| ATOM | 11260 | CA | ALA | 1672 | | -20.879 | 6.148 | | 20.20 |
| MOTA | 11261 | CB | ALA | 1672 | | -20.623 | 6.434 | | 21.78 |
| MOTA | 11262 | С | ALA " | 1672 | | -20.710 | 7.429 | | 21.55 |
| ATOM | 11263 | 0 | ALA | 1672 | 40.684 | -21.664 | 8.192 | 1.00 | 21.04 |
| MOTA | 11264 | N | ALA | 1673 | 40.382 | -19.492 | 7.654 | 1.00 | 19.63 |
| ATOM | 11265 | CA | ALA | 1673 | | -19.175 | 8.831 | | 19.73 |
| ATOM | 11266 | CB | ALA | 1673 | | -17.665 | 8.952 | | 18.51 |
| MOTA | 11267 | C | ALA | 1673 | | -19.857 | 8.782 | | 20.99 |
| MOTA | 11268 | 0 | ALA | 1673 | | -20.010 | 9.807 | | 19.73 |
| ATOM | 11269 | N | GLY | 1674 | | -20.010 | 7.584 | | 20.06 |
| | | | | | | | | | 19.89 |
| ATOM | 11270 | CA | GLY | 1674 | 30.310 | -20.928 | 7.453 | 1.00 | 12.03 |

| ATOM | 11271 | С | GLY | 1674 | 35.552 | -20.324 | 6.444 | 1.00 | 18.97 |
|--------------|----------------|----------|------------|--------------|------------------|-------------------|-------------------|------|----------------|
| ATOM | 11272 | ō | GLY | 1674 | 34.468 | -20.848 | 6.245 | 1.00 | 18.23 |
| ATOM | 11272 | N | ALA | 1675 | 35.936 | -19.217 | 5.818 | 1.00 | 19.69 |
| ATOM | 11274 | CA | ALA | 1675 | | -18.589 | 4.822 | 1.00 | |
| ATOM | 11275 | CB | ALA | 1675 | 35.736 | -17.312 | | 1.00 | |
| ATOM | 11276 | C | ALA | 1675 | 34.830 | -19.582 | 3.680 | | 21.06 |
| | 11277 | 0 | ALA | 1675 | 35.772 | -20.194 | 3.175 | | 22.86 |
| ATOM | | | | | 33.565 | -20.194 -19.741 | 3.175 | | 20.43 |
| ATOM | 11278 | N | GLN | 1676 | 33.194 | -20.659 | 2.208 | | 20.43 |
| ATOM | 11279 | CA | GLN | 1676 | | | | | |
| MOTA | 11280 | | GLN | 1676 | 31.923 | -21.426 | 2.578 | | 21.87 |
| ATOM | 11281 | CG | GLN | 1676 | 32.049 | -22.250 | 3.854 | | 23.52 |
| ATOM | 11282 | CD | GLN | 1676 | 30.805 | -23.067 | 4.165 | 1.00 | |
| ATOM | 11283 | OE1 | | 1676 | 30.470 | -24.007 | 3.449 | | 30.08 |
| ATOM | 11284 | NE2 | | 1676 | | -22.707 | 5.240 | | 28.15 |
| MOTA | 11285 | C | GLN | 1676 | | -19.938 | 0.879 | 1.00 | |
| MOTA | 11286 | 0 | GLN | 1676 | 32.822 | -20.572 | -0.163 | 1.00 | |
| MOTA | 11287 | N | LEU | 1677 | 32.973 | -18.612 | 0.928 | 1.00 | |
| MOTA | 11288 | CA | LEU | 1677 | | -17.792 | -0.257 | 1.00 | |
| MOTA | 11289 | CB | LEU | 1677 | | -17.476 | -0.467 | 1.00 | |
| ATOM | 11290 | CG | LEU | 1677 | | -18.528 | -1.225 | | 25.39 |
| MOTA | 11291 | CD1 | | 1677 | | -18.325 | -0.979 | | 26.62 |
| MOTA | 11292 | CD2 | | 1677 | 30.821 | -18.426 | -2.711 | | 25.79 |
| MOTA | 11293 | C | LEU | 1677 | 33.570 | -16.496 | -0.092 | | 21.45 |
| ATOM | 11294 | 0 | LEU | 1677 | | -16.058 | 1.030 | | 20.88 |
| ATOM | 11295 | N | LEU | 1678 | 33.944 | -15.881 | -1.210 | 1.00 | |
| ATOM | 11296 | CA | LEU | 1678 | | -14.617 | -1.168 | | 20.03 |
| MOTA | 11297 | CB | LEU | 1678 | | -14.847 | -1.284 | | 19.25 |
| MOTA | 11298 | CG | LEU | 1678 | | -13.574 | -1.442 | 1.00 | |
| MOTA | 11299 | | LEU | 1678 | | -12.699 | -0.207 | 1.00 | |
| MOTA | 11300 | CD2 | | 1678 | 38.487 | -13.937 | -1.671 | | 20.95 |
| MOTA | 11301 | C | LEU | 1678 | 34.238 | -13.695 | -2.288 | 1.00 | |
| ATOM | 11302 | 0 | LEU | 1678 | 34.090 | -14.119 | -3.432 | | 20.80 |
| ATOM | 11303 | N | VAL | 1679 | 34.026 | -12.433 | -1.947 | 1.00 | 19.50 |
| ATOM | 11304 | CA CB | VAL VAL | 1679 | | -11.435 | -2.929 -2.476 | | 20.39 |
| ATOM ATOM | 11305 11306 | | VAL | 1679 1679 | 32.202 | -10.630 -9.423 | -3.389 | | 19.05 |
| ATOM | 11307 | | VAL | 1679 | 31.145 | -11.517 | -2.518 | 1.00 | 17.14 |
| ATOM | 11307 | C | VAL | 1679 | 34.799 | -10.462 | -3.121 | | 22.00 |
| ATOM | 11300 | 0 | VAL | 1679 | 35.351 | -9.935 | -2.145 | | 20.40 |
| ATOM | 11310 | N | LEU | 1680 | 35.174 | -10.249 | -4.380 | | 22.33 |
| ATOM | 11311 | CA | LEU | 1680 | 36.250 | -9.325 | -4.745 | | 24.09 |
| ATOM | 11312 | СВ | LEU | 1680 | 37.267 | -10.011 | -5.666 | | 25.86 |
| ATOM | 11313 | CG | LEU | 1680 | 38.561 | -10.510 | -5.030 | | 28.75 |
| ATOM | 11314 | | LEU | 1,680 | 39.434 | -11.167 | -6.092 | | 28.15 |
| ATOM | 11315 | | LEU | 1680 | 39.295 | -9.338 | -4.388 | | 28.06 |
| ATOM | 11316 | С | LEU | 1680 | 35.631 | -8.147 | -5.483 | | 23.79 |
| ATOM | 11317 | 0 | LEU | 1680 | 34.984 | -8.338 | -6.508 | | 26.35 |
| ATOM | 11318 | N | GLU | 1681 | 35.829 | -6.934 | -4.976 | 1.00 | 23.88 |
| ATOM | 11319 | CA | GLU | 1681 | 35.252 | -5.753 | -5.613 | | 26.33 |
| ATOM | 11320 | СВ | GLU | 1681 | 34.293 | -5.065 | -4.636 | | 23.82 |
| ATOM | 11321 | CG | GLU | 1681 | 33.793 | -3.695 | -5.074 | 1.00 | 25:12 |
| ATOM | 11322 | CD | GLU | 1681 | 32.590 | -3.233 | -4.264 | | 25.80 |
| ATOM | 11323 | | GLU | 1681 | 32.420 | -3.717 | -3.125 | | 26.14 |
| MOTA | 11324 | | GLU | 1681 | 31.820 | -2.386 | -4.760 | 1.00 | 27.76 |
| MOTA | 11325 | С | GLU | 1681 | 36.272 | -4.742 | -6.137 | 1.00 | 27.77 |
| MOTA | 11326 | 0 | GLU | 1681 | 37.181 | -4.327 | -5.417 | 1.00 | 28.68 |
| MOTA | 11327 | N | CYS | 1682 | 36.107 | -4.354 | -7.399 | 1.00 | 29.09 |
| MOTA | 11328 | CA | CYS | 1682 | 36.982 | -3.378 | -8.045 | 1.00 | 30.51 |
| ATOM | 11329 | CB | CYS | 1682 | 36.562 | -1.968 | -7.639 | 1.00 | 30.60 |
| MOTA | 11330 | SG | CYS | 1682 | 34.887 | -1.555 | -8.174 | 1.00 | 32.38 |
| MOTA | 11331 | С | CYS | 1682 | 38.463 | -3.582 | -7.760 | | 31.19 |
| MOTA | 11332 | 0 | CYS | 1682 | 39.075 | -2.841 | -6.984 | | 32.08 |
| MOTA | 11333 | N | VAL | 1683 | 39.029 | -4.593 | -8.405 | | 31.35 |
| MOTA | 11334 | CA | VAL | 1683 | 40.436 | -4.922 | -8.248 | | 32.78 |
| ATOM | 11335 | CB | VAL | 1683 | 40.600 | -6.146 | -7.312 | | 33.52 |
| ATOM | 11336 | | VAL | 1683 | 40.443 | -7.443 | -8.094 | | 33.50 |
| ATOM | 11337 | | VAL | 1683 | 41.927 | -6.085 | -6.596 | | 34.74 |
| ATOM | 11338 | C | VAL | 1683 | 40.971 | -5.249 | -9.645 | | 33.45 |
| MOTA | 11339 | 0 | VAL | 1683 | 40.218 | | -10.516 | | 33.44 |
| MOTA | 11340 | N | PRO | 1684 | 42.274 | -5.024 | -9.887 | | 33.91 |
| MOTA | 11341 | CD | PRO | 1684 | 43.339 | -4.567 -5.330 | -8.979 -11.216 | | 33.50 33.77 |
| ATOM ATOM | 11342 11343 | CA CB | PRO | 1684 | 42.817 44.307 | | -11.216 | | 34.17 |
| ATOM | 11343 | CG | PRO PRO | 1684 1684 | 44.558 | -5.205 | -9.598 | | 34.17 |
| ATOM | 11344 | CG | PRO | 1684 | 44.558 | | -11.595 | | 33.67 |
| MOTA | 11345 | o | PRO | 1684 | 42.807 | | -10.806 | | 33.93 |
| ATOM | 11347 | N | VAL | 1685 | 42.043 | | -12.802 | | 33.35 |
| | | | | | | | | | |

| MOTA | 11348 | CA | VAL | 1685 | | 41.731 | -8.321 | -13.301 | 1.00 | 33.55 |
|--------------|----------------|----------|--------------|--------------|---|--------|--------------------|---------|------|----------------|
| ATOM | 11349 | CB | VAL | 1685 | | 41.535 | -8.305 | -14.827 | 1.00 | 33.86 |
| MOTA | 11350 | CG1 | VAL | 1685 | | 40.993 | -9.650 | -15.296 | 1.00 | 33.59 |
| MOTA | 11351 | CG2 | VAL | 1685 | | 40.601 | -7.175 | -15.216 | 1.00 | 32.41 |
| MOTA | 11352 | C | VAL | 1685 | | 42.817 | -9.343 | -12.976 | 1.00 | 34.90 |
| ATOM | 11353 | 0 | VAL | 1685 | | 42.529 | -10.426 | -12.463 | | 33.21 |
| MOTA | 11354 | N | GLU | 1686 | | 44.065 | -8.994 | -13.278 | 1.00 | 36.15 |
| MOTA | 11355 | CA | GLU | 1686 | | 45.185 | -9.893 | -13.024 | 1.00 | 37.45 |
| ATOM | 11356 | CB | GLU | 1686 | | 46.512 | -9.245 | -13.449 | 1.00 | 40.77 |
| MOTA | 11357 | CG | GLU | 1686 | | 46.516 | -7.719 | -13.470 | 1.00 | 45.35 |
| MOTA | 11358 | CD | GLU | 1686 | | 45.716 | -7.144 | -14.631 | 1.00 | 47.26 |
| MOTA | 11359 | OE1 | GLU | 1686 | | 45.988 | | -15.793 | 1.00 | 48.37 |
| MOTA | 11360 | OE2 | GLU | 1686 | | 44.820 | | -14.383 | | 49.33 |
| MOTA | 11361 | C. | GLU | 1686 | | 45.259 | -10.326 | | | 35.59 |
| MOTA | 11362 | 0 | GLU | 1686 | | | -11.460 | | | 35.39 |
| MOTA | 11363 | N | LEU | 1687 | | 44.896 | | -10.656 | | 34.93 |
| MOTA | 11364 | CA | LEU | 1687 | | 44.926 | -9.743 | -9.234 | | 34.56 |
| MOTA | 11365 | CB | LEU | 1687 | | 44.773 | -8.473 | -8.400 | | 36.48 |
| MOTA | 11366 | CG | LEU | 1687 | | 45.413 | -8.477 | -7.007 | | 38.23 |
| MOTA | 11367 | | LEU | 1687 | | 45.086 | -7.168 | -6.311 | | 39.44 |
| MOTA | 11368 | | LEU | 1687 | | 44.909 | -9.646 | -6.189 | | 40.16 |
| MOTA | 11369 | С | LEU | 1687 | | 43.783 | -10.706 | -8.934 | | 33.56 |
| ATOM | 11370 | 0 | LEU | 1687 | | 43.940 | -11.656 | -8.166 | | 33.33 |
| ATOM | 11371 | N | ALA | 1688 | | | -10.455 | -9.552 | | 33.02 |
| MOTA | 11372 | CA | ALA | 1688 | | | -11.303 | -9.374 | | 32.03 |
| MOTA | 11373 | CB | ALA | 1688 | | | -10.748 | | | 31.82 |
| MOTA | 11374 | C | ALA | 1688 | | | -12.713 | -9.841 | | 31.88 |
| MOTA | 11375 | 0 | ALA | 1688 | | | -13.698 | -9.288 | | 30.38 |
| MOTA | 11376 | N | LYS | 1689 | | | -12.799 | | | 32.10 |
| ATOM | 11377 | CA | LYS | 1689 | | | -14.080 | -11.420 | | 32.59 |
| ATOM | 11378 | CB | LYS | 1689 | | | -13.852 | -12.667 | | 35.33 |
| ATOM | 11379 | CG | LYS | 1689 | | | -12.915 | | | 39.20 43.71 |
| MOTA | 11380 | CD. | LYS | 1689 | | | -12.702 -11.725 | | | 44.72 |
| MOTA | 11381 | CE NZ | LYS | 1689 1689 | | | -11.725 | | | 46.98 |
| ATOM | 11382 11383 | | LYS LYS | 1689 | | | -14.854 | -10.392 | | 30.77 |
| ATOM ATOM | 11383 | С О | LYS | 1689 | | | -16.040 | | | 30.60 |
| ATOM | 11384 | N | ARG | 1690 | | | -14.172 | -9.793 | | 30.36 |
| ATOM | 11386 | CA | ARG | 1690 | • | | -14.773 | | | 30.78 |
| ATOM | 11387 | CB | ARG | 1690 | • | | -13.738 | -8.236 | | 32.24 |
| ATOM | 11388 | CG | ARG | 1690 | | | -13.968 | -8.653 | | 35.21 |
| ATOM | 11389 | CD | ARG | 1690 | | 49.122 | -13.194 | -7.766 | | 35.72 |
| ATOM | 11390 | NE | ARG | 1690 | | 48.987 | -11.749 | -7.919 | | 38.51 |
| ATOM | 11391 | CZ. | ARG | 1690 | | | -10.854 | -7.110 | | 38.81 |
| ATOM | 11392 | | ARG | 1690 | - | | -11.253 | -6.082 | | 38.33 |
| ATOM | 11393 | | ARG | 1690 | | 49.374 | -9.557 | -7.331 | | 38.70 |
| ATOM | 11394 | С | ARG | 1690 | | | -15.329 | -7.627 | | 29.79 |
| MOTA | 11395 | Ō | ARG | 1690 | | 45.018 | -16.503 | -7.271 | | 29.49 |
| ATOM | 11396 | N | ILE | 1691 | | | -14.475 | -7.044 | | 29.53 |
| ATOM | 11397 | CA | ILE | 1691 | | 43.223 | -14.874 | -5.920 | 1.00 | 27.99 |
| ATOM | 11398 | CB. | ILE | 1691 | | 42.368 | -13.687 | -5.428 | 1.00 | 28.66 |
| ATOM | 11399 | CG2 | ILE | 1691 | | 41.431 | -14.141 | -4.310 | 1.00 | 29.07 |
| MOTA | 11400 | | ILE | 1691 | | | -12.569 | -4.939 | 1.00 | 27.59 |
| MOTA | 11401 | CD1 | ILE | 1691 | | 42.571 | -11.367 | -4.367 | 1.00 | 30.13 |
| MOTA | 11402 | С | ILE | 1691 | | 42.322 | -16.053 | -6.278 | 1.00 | 28.14 |
| MOTA | 11403 | 0 | ILE | 1691 | | 42.267 | -17.044 | -5.551 | 1.00 | 28.03 |
| ATOM | 11404 | N | THR | 1692 | | | -15.952 | -7.412 | | 27.85 |
| MOTA | 11405 | CA | THR | 1692 | | | -17.016 | -7.852 | | 28.15 |
| MOTA | 11406 | CB | THR | 1692 | | | -16.670 | -9.207 | | 27.92 |
| MOTA | 11407 | OG1 | | 1692 | | | -15.477 | -9.070 | | 30.45 |
| MOTA | 11408 | | THR | 1692 | | | -17.799 | -9.672 | | 24.79 |
| ATOM . | 11409 | С | THR | 1692 | | | -18.352 | -7.975 | | 28.88 |
| ATOM | 11410 | 0 | THR | 1692 | | | -19.378 | -7.523 | | 27.96 |
| ATOM | 11411 | N | GLU | 1693 | | | -18.346 | -8.585 | | 30.86 |
| ATOM | 11412 | CA | GLU | 1693 | | • | -19.582 | -8.739 | | 31.66 |
| ATOM | 11413 | CB | GLU | 1693 | | | -19.403 | -9.788 | | 34.46 |
| MOTA | 11414 | CG | GLU | 1693 | | | -19.142 | | | 39.25 |
| ATOM | 11415 | CD | GLU | 1693 | | | -18.913 | -12.193 | | 41.31 |
| ATOM | 11416 | | GLU | 1693 | | | -17.920 | | | 42.03 |
| ATOM | 11417 | | GLU | 1693 | | | -19.728 -20.022 | -13.133 | | 44.22 31.18 |
| ATOM | 11418 | C | GLU | 1693 | | | -20.022 | -7.417 | | 32.59 |
| ATOM ATOM | 11419 11420 | O N | GLU . ALA | 1693 1694 | | | -19.055 | -6.556 | | 29.06 |
| ATOM | 11420 | CA | ALA ALA | 1694 | | | -19.033 | | | 28.83 |
| ATOM | 11421 | CB | ALA | 1694 | | | -18.077 | -4.681 | | 28.10 |
| ATOM | | ·C | ALA | 1694 | | | -19.975 | -4.252 | | 28.71 |
| ATOM | 11424 | 0 | ALA | 1694 | | | -20.833 | -3.463 | | 27.81 |
| | | - | | | | | | | | |

| ATOM | 11425 | N | LEU | 1695 | | 42.734 | -19.556 | -4.273 | 1.00 28.34 |
|--------------|----------------|-------|-----|------|---|--------|--------------------|---------|--------------------------|
| ATOM | 11426 | CA | LEU | 1695 | | | -20.103 | -3.336 | 1.00 28.55 |
| | | | | | | | | | |
| MOTA | 11427 | CB | LEU | 1695 | | | -19.035 | -2.936 | 1.00 28.01 |
| MOTA | 11428 | CG | LEU | 1695 | | | -17.849 | -2.121 | 1.00 30.89 |
| ATOM | 11429 | CD1 | LEU | 1695 | | 40.062 | -16.980 | -1.700 | 1.00 27.57 |
| MOTA | 11430 | CD2 | LEU | 1695 | | 41.989 | -18.348 | -0.898 | 1.00 32.34 |
| MOTA | 11431 | C | LEU | 1695 | | 41.002 | -21.306 | -3.889 | 1.00 26.44 |
| ATOM | 11432 | 0 | LEU | 1695 | | | -21.452 | -5.099 | 1.00 27.20 |
| ATOM | 11433 | N | ALA | 1696 | | | -22.168 | -2.991 | 1.00 24.30 |
| | | | | | | | -23.346 | | 1.00 23.55 |
| ATOM | 11434 | CA | ALA | 1696 | | | | -3.391 | |
| MOTA | 11435 | CB | ALA | 1696 | | | -24.479 | -2.413 | 1.00 21.99 |
| MOTA | 11436 | С | ALA | 1696 | | | -22.983 | -3.416 | 1.00 23.10 |
| ATOM . | . 11437 | 0 | ALA | 1696 | | 37.562 | -23.440 | -4.279 | 1.00 24.16 |
| ATOM | 11438 | N | ILE | 1697 | | 37.898 | -22.155 | -2.464 | 1.00 21.53 |
| MOTA | 11439 | CA | ILE | 1697 | | 36.506 | -21.734 | -2.391 | 1.00 20.71 |
| ATOM | 11440 | CB | ILE | 1697 | | | -20.965 | -1.082 | 1.00 18.95 |
| ATOM | 11441 | CG2 | ILE | 1697 | | | -21.897 | 0.113 | 1.00 17.11 |
| | 11442 | CG1 | ILE | 1697 | | | -19.776 | -0.955 | 1.00 17.11 |
| MOTA | | | | | | | | | |
| MOTA | 11443 | CD1 | | 1697 | | | -18.806 | 0.147 | 1.00 20.97 |
| MOTA | 11444 | С | ILE | 1697 | | | -20.823 | -3.571 | 1.00 20.34 |
| MOTA | 11445 | 0 | ILE | 1697 | | 37.073 | -20.206 | -4.155 | 1.00 20.05 |
| MOTA | 11446 | N | PRO | 1698 | | 34.903 | -20.739 | -3.948 | 1.00 21.40 |
| ATOM | 11447 | CD | PRO | 1698 | | 33.767 | -21.568 | -3.513 | 1.00 20.73 |
| ATOM | 11448 | CA | PRO | 1698 | | | -19.878 | -5.074 | 1.00 20.26 |
| ATOM | 11449 | СВ | PRO | 1698 | | | -20.302 | -5.393 | 1.00 21.48 |
| | | CG | | 1698 | | | -20.847 | -4.113 | 1.00 22.95 |
| MOTA | 11450 | | PRO | | | | | | |
| ATOM | 11451 | C | PRO | 1698 | | | -18.390 | -4.769 | 1.00 20.91 |
| ATOM | 11452 | 0 | PRO | 1698 | | | -17932 | -3.650 | 1.00 19.65 |
| ATOM | 11453 | N | VAL | 1699 | | 35.138 | -17.648 | -5.770 | 1.00 18.53 |
| ATOM | 11454 | CA | VAL | 1699 | | 35.337 | -16.216 | -5.637 | 1.00 19.92 |
| ATOM | 11455 | CB | VAL | 1699 | | 36.802 | -15.840 | -5.991 | 1.00 20.40 |
| ATOM | 11456 | | VAL | 1699 | | 37.002 | -14.335 | -5.923 | 1.00 18.70 |
| ATOM | 11457 | CG2 | VAL | 1699 | | | -16.534 | -5.028 | 1.00 18.50 |
| ATOM | 11458 | C | VAL | 1699 | | | -15.480 | -6.560 | 1.00 21.83 |
| | | | | | | | | | |
| ATOM | 11459 | 0 | VAL | 1699 | | | -15.672 | -7.779 | 1.00 22.52 |
| ATOM | 11460 | N | ILE | 1700 | | | -14.648 | -5.967 | 1.00 22.27 |
| MOTA | 11461 | CA | ILE | 1700 | | | -13.886 | -6.722 | 1.00 22.16 |
| MOTA | 11462 | CB | ILE | 1700 | | 31.211 | -13.759 | -5.940 | 1.00 21.79 |
| MOTA | 11463 | CG2 | ILE | 1700 | | 30.243 | -12.873 | -6.700 | 1.00 22.27 |
| MOTA | 11464 | CG1 | ILE | 1700 | | 30.617 | -15.150 | -5.709 | 1.00 22.01 |
| ATOM | 11465 | CD1 | ILE | 1700 | | | -15.157 | -4.789 | 1.00 24.61 |
| ATOM | 11466 | c | ILE | 1700 | - | | -12.504 | -6.963 | 1.00 21.79 |
| ATOM | 11467 | | ILE | 1700 | | | -11.828 | -6.030 | 1.00 21.47 |
| | | 0 | | | | | | | |
| MOTA | 11468 | N | GLY | 1701 | | | -12.079 | -8.218 | 1.00 21.16 |
| MOTA | 11469 | CA | GLY | 1701 | | | -10.773 | -8.526 | 1.00 20.63 |
| MOTA | 11470 | С | GLY | 1701 | | 32.633 | -9.714 | -8.929 | 1.00 21.51 |
| MOTA | 11471 | 0 | GLY | 1701 | | 31.571 | -10.003 | -9.467 | 1.00 22.89 |
| ATOM | 11472 | N | ILE | 1702 | | 32.990 | -8.470 | -8.642 | 1.00 24.15 |
| ATOM | 11473 | CA | ILE | 1702 | | 32.184 | -7.309 | -8.988 | 1.00 25.08 |
| ATOM | 11474 | СВ | ILE | 1702 | | 31.275 | -6.866 | -7.804 | 1.00 25.11 |
| MOTA | 11475 | | ILE | 1702 | | 32.059 | -6.838 | -6.504 | 1.00 24.79 |
| | | | ILE | | | | -5.490 | | |
| | 11476 | | | | | | | | |
| ATOM | 11477 | | ILE | 1702 | | 29.632 | -5.485 | -9.157 | 1.00 30.16 |
| MOTA | 11478 | C | ILE | 1702 | | 33.209 | -6.228 | -9.321 | 1.00 25.61 |
| ATOM | 11479 | 0 | ILE | 1702 | | 33.728 | -5.553 | -8.437 | 1.00 25.75 |
| ATOM | 11480 | N | GLY | 1703 | | 33.515 | | -10.608 | 1.00 27.06 |
| ATOM | 11481 | CA | GLY | 1703 | | 34.501 | -5.105 | -11.017 | 1.00 24.09 |
| ATOM | 11482 | С | GLY | 1703 | | 35.884 | -5.717 | -10.904 | 1.00 25.54 |
| MOTA | 11483 | 0 | GLY | 1703 | | 36.873 | | -10.680 | 1.00 27.11 |
| ATOM | 11484 | N | ALA | 1704 | | 35.945 | | -11.054 | 1.00 24.77 |
| MOTA | 11485 | CA | ALA | 1704 | | 37.204 | | -10.970 | 1.00 24.77 |
| | | | | | | | | | |
| ATOM | 11486 | CB | ALA | 1704 | | 37.187 | -8.691 | -9.757 | 1.00 24.95 |
| ATOM | 11487 | С | ALA | 1704 | | 37.454 | | -12.238 | 1.00 26.93 |
| MOTA | 11488 | 0 | ALA | 1704 | | 38.294 | | -12.250 | 1.00 27.02 |
| MOTA | 11489 | N | GLY | 1705 | | 36.725 | | -13.303 | 1.00 27.42 |
| MOTA | 11490 | CA | GLY | 1705 | | 36.895 | -8.993 | -14.545 | 1.00 27.32 |
| MOTA | 11491 | С | GLY | 1705 | | 36.120 | -10.297 | -14.548 | 1.00 27.69 |
| ATOM | . 11492 | 0 | GLY | 1705 | | | -10.653 | | 1.00 28.16 |
| ATOM | 11493 | N | ASN | 1706 | | | -11.017 | | 1.00 26.41 |
| ATOM | 11494 | CA | ASN | 1706 | | | -12.279 | | 1.00 26.15 |
| | | | | | | | -12.423 | | 1.00 28.81 |
| ATOM | 11495 | CB | ASN | 1706 | | | | | |
| ATOM | 11496 | CG | ASN | 1706 | | | -12.410 | | 1.00 30.05 |
| ATOM | 11497 | | ASN | 1706 | | | -12.663 | | 1.00 32.36 |
| | | KID 2 | ASN | 1706 | | 37.231 | -12.111 | -17.866 | 1.00 27.42 |
| MOTA | 11498 | NDZ | | | | | | | |
| ATOM ATOM | 11498 11499 | C | ASN | 1706 | | 36.306 | -13.492 | -15.452 | 1.00 27.06 |
| | | | | | | | -13.492 -14.609 | | 1.00 27.06 1.00 28.09 |
| ATOM | 11499 | С | ASN | 1706 | | 36.005 | -14.609 | | 1.00 28.09 |

| ATOM | 11502 | CA | VAL | 1707 | 38.270 | -14.335 | -14.258 | 1.00 27.59 |
|--------------|----------------|-----------|------------|--------------|------------------|--------------------|--------------------|--------------------------|
| MOTA | 11503 | CB | VAL | 1707 | 39.700 | -13.780 | -14.047 | 1.00 29.11 |
| MOTA | 11504 | CG1 | VAL | 1707 | 40.656 | -14.914 | -13.711 | 1.00 33.83 |
| MOTA | 11505 | CG2 | VAL | 1707 | 40.169 | -13.053 | -15.299 | 1.00 30.80 |
| MOTA | 11506 | C | VAL | 1707 | 37.815 | -15.016 | -12.967 | 1.00 26.92 |
| ATOM | 11507 | 0 | LAV | 1707 | | -16.088 | | 1.00 26.60 |
| ATOM | 11508 | N | THR | 1708 | | -14.389 | | 1.00 24.26 |
| MOTA | 11509 | CA | THR | 1708 | 36.364 | -14.948 | -11.019 | 1.00 23.16 |
| ATOM | 11510 | CB | THR | 1708 | 35.625 | -13.867 | -10.202 | 1.00 22.08 |
| MOTA | 11511 | OG1 | THR | 1708 | | -13.145 | | 1.00 20.76 |
| MOTA | 11512 | CG2 | THR | 1708 | | -12.894 | -9.592 | 1.00 22.51 |
| MOTA | 11513 | C | THR | 1708 | | -16.122 | | 1.00 23.44 |
| MOTA | 11514 | 0 | THR | 1708 | | -16.304 | | 1.00 24.03 |
| MOTA | 11515 | N | ASP | 1709 | | -16.921 | | 1.00 23.18 |
| MOTA | 11516 | CA | ASP | 1709 | | -18.098 | | 1.00 24.19 |
| MOTA | 11517 | CB | ASP | 1709 | | -18.954 | -9.139 | 1.00 26.39 |
| ATOM | 11518 | CG | ASP | 1709 | | -19.362 | -8.861 | 1.00 28.72 |
| MOTA | 11519 | | ASP | 1709 | | -20.179 | -9.636 | 1.00 28.85 |
| ATOM | 11520 | | ASP | 1709 | | -18.858 | -7.876 | 1.00 27.39 |
| ATOM | 11521 | C | ASP | 1709 | | -17.708 | | 1.00 24.34 |
| MOTA | 11522 | 0 | ASP | 1709 | | -18.461 | | 1.00 23.59 |
| MOTA | 11523 | N | GLY | 1710 | | -16.521 -16.032 | | 1.00 22.85 1.00 21.26 |
| ATOM | 11524 | CA | GLY GLY | 1710 1710 | | -14.522 | | 1.00 21.20 |
| ATOM ATOM | 11525 11526 | C O | GLY | 1710 | | -13.878 | | 1.00 13.07 |
| ATOM | 11527 | N | GLN | 1711 | | -13.956 | | 1.00 18.22 |
| ATOM | 11527 | CA | GLN | 1711 | | -12.510 | | 1.00 18.74 |
| ATOM | 11529 | CB. | GLN | 1711 | | -12.074 | | 1.00 18.46 |
| ATOM | 11530 | CG . | GLN | 1711 | | -12.373 | | 1.00 15.95 |
| ATOM | 11531 | CD | GLN | 1711 | | -11.589 | | 1.00 19.23 |
| MOTA | 11532 | | GLN | 1711 | | -10.409 | | 1.00 20.10 |
| ATOM | 11532 | NE2 | GLN | 1711 | | -12.237 | | 1.00 21.35 |
| ATOM | 11534 | C | GLN | 1711 | | -12.056 | -9.712 | 1.00 19.28 |
| ATOM | 11535 | 0 | GLN | 1711 | | -12.852 | -9.359 | 1.00 18.49 |
| ATOM | 11536 | N | ILE | 1712 | | -10.767 | -9.401 | 1.00 21.16 |
| ATOM | 11537 | CA | ILE | 1712 | | -10.172 | -8.634 | 1.00 23.23 |
| ATOM | 11538 | СВ | ILE | 1712 | 27.772 | -10.262 | -7.109 | 1.00 24.48 |
| ATOM | 11539 | CG2 | ILE | 1712 | 28.930 | -9.342 | -6.706 | 1.00 25.08 |
| ATOM | 11540 | CG1 | ILE | 1712 | 26.492 | -9.870 | -6.365 | 1.00 25.35 |
| MOTA | 11541 | CD1 | ILE | 1712 | 26.463 | -10.280 | -4.898 | 1.00 29.02 |
| MOTA | 11542 | C | ILE | 1712 | 27.374 | -8.710 | -9.055 | 1.00 24.32 |
| MOTA | 11543 | 0 | ILE | 1712 | 28.328 | -8.085 | -9.539 | 1.00 23.00 |
| ATOM | 11544 | N | LEU | 1713 | 26.172 | -8.169 | -8.888 | 1.00 24.37 |
| MOTA | 11545 | CA | LEU | 1713 | 25.914 | -6.778 | -9.249 | 1.00 27.03 |
| ATOM | 11546 | CB | LEU | 1713 | 25.837 | | -10.772 | 1.00 30.07 |
| ATOM | 11547 | CG | LEU | 1713 | 26.489 | | -11.427 | 1.00 33.56 |
| MOTA | 11548 | | LEU | 1713 | 26.318 | | -12.934 | 1.00 36.19 |
| MOTA | 11549 | CD2 | LEU | 1713 | 25.851 | | -10.908 | 1.00 36.32 |
| ATOM | 11550 | C | LEU | 1713 | 24.609 | -6.296 | -8.620 | 1.00 26.45 |
| MOTA | 11551 | 0 | LEU | 1713 | 23.723 | -7.099 -4.989 | -8.338 -8.386 | 1.00 23.98 1.00 25.79 |
| ATOM | 11552 11553 | N | VAL | 1714 1714 | 24.509 23.299 | | -7.808 | 1.00 25.79 |
| ATOM | | CA | VAL VAL | 1714 | 23.522 | ~2.943 | -7.363 | 1.00 25.33 |
| ATOM ATOM | 11554 11555 | CB CG1 | VAL | 1714 | 22.245 | -2.343 | -6.750 | 1.00 25.51 |
| ATOM | 11556 | CG2 | VAL | 1714 | 24.660 | -2.878 | -6.351 | 1.00 27.39 |
| ATOM | 11557 | C | VAL | 1714 | 22.215 | -4.466 | -8.886 | 1.00 24.33 |
| ATOM | 11558 | Õ | VAL | 1714 | 22.3.79 | -3.913 | -9.978 | 1.00 21.59 |
| ATOM | 11559 | N | MET · | 1715 | 21.115 | -5.146 | -8.573 | 1.00 22.29 |
| ATOM | 11560 | CA | MET | 1715 | 20.026 | ~5.302 | -9.521 | 1.00 20.64 |
| ATOM | 11561 | CB | MET | 1715 | 18.855 | -6.059 | -8.881 | 1.00 18.66 |
| ATOM | 11562 | CG | MET | 1715 | 18.253 | -5.362 | -7.667 | 1.00 16.03 |
| MOTA | 11563 | SD | MET | 1715 | 16.444 | -5.523 | -7.565 | 1.00 14.77 |
| ATOM | 11564 | CE | MET | 1715 | 15.937 | -4.242 | -8.684 | 1.00 11.94 |
| MOTA | 11565 | С | MET | 1715 | 19.519 | -3.983 | -10.101 | 1.00 19.82 |
| MOTA | 11566 | 0 | MET | 1715 | 19.002 | | -11.213 | 1.00 21.61 |
| MOTA | 11567 | N | HIS | 1716 | 19.668 | -2.890 | -9.364 | 1.00 19.03 |
| MOTA | 11568 | CA | HIS | 1716 | 19.192 | -1.600 | -9.855 | 1.00 22.19 |
| MOTA | 11569 | CB | HIS | 1716 | 19.137 | -0.596 | -8.703 | 1.00 20.78 |
| MOTA | 11570 | CG | HIS | 1716 | 18.098 | -0.932 | -7.675 | 1.00 21.06 |
| MOTA | 11571 | | HIS | 1716 | 18.126 | -1.784 | -6.623 | 1.00 18.32 |
| ATOM | 11572 | | HIS | 1716 | 16.826 | -0.399 | -7.699 | 1.00 20.68 |
| ATOM | 11573 | | HIS | 1716 | 16.116 | -0.907 | -6.707 | 1.00 18.23 |
| ATOM | 11574 | | HIS | 1716 | 16.882 | -1.750 | -6.039 | 1.00 21.81 |
| MOTA | 11575 | C | HIS | 1716 | 20.035 | | -11.018 | 1.00 22.57 |
| ATOM | 11576 | O N | HIS | 1716 | 19.558 21.287 | | -11.835 -11.097 | 1.00 22.73 1.00 23.70 |
| MOTA MOTA | 11577 11578 | N | ASP | 1717 | 22.145 | | -12.199 | 1.00 25.70 |
| 71 OH | 117/0 | CA | ASP | 1717 | 22.143 | 1.009 | 10.173 | 1.00 20.03 |

| ATOM | 11579 | CB | ASP | 1717 | 23.615 | -1.081 -11.769 | 1.00 27.37 |
|---------|----------------|----------|------------|--------------|--------|----------------|------------|
| MOTA | 11580 | CG | ASP | 1717 | 23.891 | -0.070 -10.672 | 1.00 27.23 |
| ATOM | 11581 | | ASP | 1717 | 23.334 | 1.040 -10.740 | 1.00 28.27 |
| | | | | 1717 | 24.663 | -0.386 -9.748 | 1.00 27.57 |
| MOTA | 11582 | | ASP | | | | |
| ATOM | 11583 | С | ASP | 1717 | 21.939 | -2.064 -13.353 | 1.00 27.25 |
| MOTA | 11584 | 0 | ASP | 1717 | 22.022 | -1.687 -14.522 | 1.00 26.75 |
| MOTA | 11585 | N | ALA | 1718 | 21.641 | -3.315 -13.013 | 1.00 26.99 |
| ATOM | 11586 | CA | ALA | 1718 | 21.424 | -4.349 -14.019 | 1.00 28.53 |
| ATOM | 11587 | CB | ALA | 1718 | 21.320 | -5.716 -13.344 | 1.00 28.27 |
| ATOM | 11588 | C | ALA | 1718 | 20.196 | -4.099 -14.896 | 1.00 28.41 |
| | 11589 | ō | ALA | 1718 | 20.106 | -4.644 -15.995 | 1.00 29.83 |
| ATOM | | | | | | -3.278 -14.422 | |
| MOTA | 11590 | N | PHE | 1719 | 19.258 | | 1.00 30.20 |
| ATOM | 11591 | CA | PHE | 1719 | 18.053 | -2.968 -15.197 | 1.00 29.35 |
| MOTA | 11592 | CB | PHE | 1719 | 16.797 | -3.436 -14.458 | 1.00 30.92 |
| ATOM | 11593 | CG ` | PHE | 1719 | 16.863 | -4.866 -14.004 | 1.00 31.07 |
| MOTA | 11594 | CD1 | PHE | 1719 | 17.299 | -5.863 -14.870 | 1.00 34.00 |
| MOTA | 11595 | CD2 | PHE | 1719 | 16.500 | -5.215 -12.708 | 1.00 33.37 |
| ATOM | 11596 | | PHE | 1719 | 17.379 | -7.187 -14.453 | 1.00 33.82 |
| | 11597 | | PHE | 1719 | 16.574 | -6.537 -12.278 | 1.00 34.22 |
| MOTA | | | | | | | |
| MOTA | 11598 | CZ | PHE | 1719 | 17.016 | -7.524 -13.155 | 1.00 35.15 |
| MOTA | 11599 | С | PHE | 1719 | 17.912 | -1.484 -15.533 | |
| MOTA | 11600 | 0 | PHE | 1719 | 16.837 | -1.021 -15.919 | 1.00 29.75 |
| ATOM | 11601 | N | GLY | 1720 | 18.999 | -0.738 -15.391 | 1.00 30.77 |
| MOTA | 11602 | CA | GLY | 1720 | 18.955 | 0.680 -15.699 | 1.00 29.22 |
| ATOM | 11603 | С | GLY | 1720 | 17.997 | 1.486 -14.839 | 1.00 29.76 |
| ATOM | 11604 | ō | GLY | 1720 | 17.524 | 2.546 -15.258 | 1.00 30.07 |
| | | | | | 17.701 | 0.998 -13.638 | 1.00 25.96 |
| MOTA | 11605 | N | ILE | 1721 | | | |
| ATOM | 11606 | CA | ILE . | | 16.806 | 1.721 -12.743 | 1.00 25.33 |
| MOTA | 11607 | CB | ILE | 1721 | 16.312 | 0.817 -11.572 | 1.00 21.96 |
| MOTA | 11608 | CG2 | ILE | 1721 | 15.463 | 1.629 -10.606 | 1.00 22.06 |
| ATOM | 11609 | CG1 | ILE | 1721 | 15.492 | -0.352 -12.118 | 1.00 23.00 |
| ATOM | 11610 | CD1 | ILE | 1721 | 15.126 | -1.395 -11.081 | 1.00 22.54 |
| ATOM | 11611 | С | ILE | 1721 | 17.530 | 2.940 -12.168 | 1.00 25.41 |
| ATOM | 11612 | ō | ILE | 1721 | 16.960 | 4.020 -12.089 | 1.00 25.23 |
| | | | | | | 2.766 -11.778 | 1.00 28.45 |
| ATOM | 11613 | N | THR | 1722 | 18.792 | | |
| MOTA | 11614 | CA | THR | 1722 | 19.563 | 3.871 -11.206 | 1.00 31.68 |
| ATOM | 11615 | CB | THR | 1722 | 20.885 | 3.387 -10.588 | 1.00 31.93 |
| MOTA | 11616 | OG1 | THR | 1722 | 21.778 | 2.969 -11.626 | 1.00 35.74 |
| ATOM | 11617 | CG2 | THR | 1722 | 20.634 | 2.227 -9.643 | 1.00 28.90 |
| ATOM | 11618 | С | THR | 1722 | 19.895 | 4.940 -12.243 | 1.00 34.83 |
| ATOM | 11619 | O | THR | 1722 | 20.220 | 4.621 -13.386 | 1.00 34.13 |
| ATOM | 11620 | N | GLY | 1723 | 19.811 | 6.200 -11.816 | 1.00 38.15 |
| | | | | 1723 | 20.100 | 7.342 -12.667 | 1.00 44.26 |
| ATOM | 11621 | CA | GLY | | | | |
| ATOM | 11622 | С | GLY | 1723 | 20.393 | 7.053 -14.126 | 1.00 48.27 |
| ATOM | 11623 | 0 | GLY | 1723 | 19.534 | 6.554 -14.857 | 1.00 50.07 |
| ATOM | 11624 | N | GLY | 1724 | 21.612 | 7.368 -14.554 | 1.00 50.26 |
| ATOM | 11625 | CA | GLY | 1724 | 21.990 | 7.136 -15.936 | 1.00 52.51 |
| MOTA | 11626 | С | GLY | 1724 | 23.414 | 6.641 -16.078 | 1.00 54.09 |
| ATOM | 11627 | 0 | GLY | 1724 | 23.677 | 5.698 -16.825 | 1.00 55.33 |
| ATOM | 11628 | N | HIS | 1725 | 24.338 | 7.275 -15.363 | 1.00 55.09 |
| ATOM | 11629 | CA | HIS | 1725 | 25.742 | 6.881 -15.429 | 1.00 56.44 |
| | | | | | | | |
| MOTA | 11630 | CB | HIS | 1725 | 26.648 | 8.096 -15.214 | 1.00 58.71 |
| MOTA | 11631 | CG | HIS | 1725 | 26.616 | 9.079 -16.342 | 1.00 61.40 |
| MOTA | 11632 | | HIS | 1725 | 26.415 | 10.418 -16.354 | 1.00`62.22 |
| MOTA | 11633 | ND1 | HIS | 1725 | 26.821 | 8.711 -17.654 | 1.00 62.27 |
| MOTA | 11634 | | HIS | 1725 | 26.748 | 9.780 -18.426 | 1.00 63.11 |
| ATOM | 11635 | NE2 | HIS | 1725 | 26.503 | 10.829 -17.662 | 1.00 63.16 |
| MOTA | 11636 | С | HIS | 1725 | 26.097 | 5.797 -14.419 | 1.00 55.56 |
| ATOM | 11637 | 0 | HIS | 1725 | 26.673 | 6.078 -13.369 | 1.00 55.59 |
| ATOM | 11638 | N | ILE | 1726 | 25.754 | 4.555 -14.748 | 1.00 54.42 |
| | 11639 | CA | ILE | 1726 | 26.044 | 3.425 -13.875 | 1.00 53.21 |
| ATOM | | | | | | | |
| ATOM | 11640 | CB | ILE | 1726 | 25.356 | 2.134 -14.382 | 1.00 53.76 |
| MOTA | 11641 | CG2 | ILE | 1726 | 23.843 | 2.277 -14.290 | 1.00 53.32 |
| MOTA | 11642 | CG1 | ILE | 1726 | 25.788 | 1.845 -15.822 | 1.00 54.09 |
| ATOM | 11643 | CD1 | ILE | 1726 | 25.277 | 0.524 -16.365 | 1.00 53.89 |
| MOTA | 11644 | С | ILE | 1726 | 27.554 | 3.195 -13.821 | 1.00 51.83 |
| ATOM | 11645 | 0 | ILE | 1726 | 28.297 | 3.700 -14.665 | 1.00 51.84 |
| ATOM | 11646 | N | PRO | 1727 | 28.029 | 2.431 -12.825 | 1.00 49.69 |
| ATOM | 11647 | CD | PRO | 1727 | 27.283 | 1.702 -11.785 | 1.00 49.25 |
| ATOM | 11648 | CA | PRO | 1727 | 29.468 | 2.172 -12.715 | 1.00 48.30 |
| | | | | | | 1.318 -11.453 | 1.00 48.75 |
| ATOM | 11649 | CB | PRO | 1727 | 29.566 | | |
| MOTA | 11650 | CG | PRO | 1727 | 28.250 | 0.611 -11.416 | 1.00 49.22 |
| ATOM | 11651 | С | PRO | 1727 | 30.040 | 1.480 -13.953 | 1.00 46.66 |
| MOTA | 11652 | 0 | PRO | 1727 | 29.368 | 0.669 -14.589 | 1.00 46.75 |
| MOTA | 11653 | N | LYS | 1728 | 31.283 | 1.808 -14.290 | 1.00 44.70 |
| 2 ELONA | | | | | 24 242 | 1 222 15 457 | 1 00 42 21 |
| MOTA | 11654 | CA | LYS | 1728 | 31.940 | 1.230 -15.457 | 1.00 42.31 |
| ATOM | 11654 11655 | CA CB | LYS LYS | 1728 1728 | 31.940 | 1.747 -15.571 | 1.00 42.31 |

| ATOM | 11656 | CG | LYS | 1728 | 33.500 | 3.186 -16.065 | 1.00 49.29 |
|------|-------|-----|-----|--------|--------|----------------|------------|
| ATOM | 11657 | CD | LYS | 1728 | 32.922 | 4.188 -15.074 | 1.00 51.69 |
| MOTA | 11658 | CE | LYS | 1728 | 33.050 | 5.614 -15.598 | 1.00 52.92 |
| ATOM | 11659 | NZ | LYS | 1728 | 32.499 | 6.622 -14.646 | 1.00 54.39 |
| ATOM | 11660 | C | LYS | 1728 | 31.954 | -0.293 -15.470 | 1.00 38.59 |
| | 11661 | Ö | LYS | 1728 | 31.994 | -0.906 -16.536 | 1.00 37.57 |
| MOTA | | | | | | | 1.00 37.57 |
| MOTA | 11662 | N | PHE | 1729 | 31.920 | -0.904 -14.292 | |
| MOTA | 11663 | CA | PHE | 1729 | 31.947 | -2.358 -14.201 | 1.00 30.76 |
| MOTA | 11664 | CB | PHE | 1729 | 32.582 | -2.782 -12.870 | 1.00 31.47 |
| MOTA | 11665 | CG | PHE | 1729 | 31.882 | -2.234 -11.657 | 1.00 31.03 |
| ATOM | 11666 | CD1 | PHE | 1729 | 30.666 | -2.765 -11.232 | 1.00 31.72 |
| ATOM | 11667 | CD2 | PHE | 1729 | 32.445 | -1.190 -10.932 | 1.00 31.83 |
| ATOM | 11668 | CE1 | PHE | 1729 | 30.027 | -2.265 -10.099 | 1.00 30.43 |
| MOTA | 11669 | CE2 | PHE | 1729 | 31.816 | -0.684 -9.800 | 1.00 32.00 |
| ATOM | 11670 | CZ | PHE | 1729 | 30.604 | -1.222 -9.381 | 1.00 32.08 |
| ATOM | 11671 | C | PHE | 1729 | 30.571 | -2.999 -14.346 | 1.00 27.80 |
| ATOM | 11672 | ō | PHE | 1729 | 30.460 | -4.215 -14.486 | 1.00 26.63 |
| ATOM | 11673 | N | ALA | 1730 | 29.526 | -2.181 -14.321 | 1.00 26.96 |
| | | | | 1730 | 28.165 | -2.694 -14.435 | 1.00 26.38 |
| ATOM | 11674 | CA | ALA | | | -1.938 -13.486 | 1.00 25.85 |
| ATOM | 11675 | CB | ALA | 1730 | 27.243 | | |
| MOTA | 11676 | C | ALA | 1730 | 27.627 | -2.611 -15.852 | 1.00 26.64 |
| MOTA | 11677 | 0 | ALA | 1730 | 28.155 | -1.886 -16.694 | 1.00 27.21 |
| MOTA | 11678 | N | LYS | 1731 | 26.565 | -3.362 -16.112 | 1.00 25.32 |
| MOTA | 11679 | CA | LYS | 1731 | 25.951 | -3.348 -17.427 | 1.00 26.32 |
| MOTA | 11680 | CB | LYS | 1731 | 26.419 | -4.550 -18.241 | 1.00 27.13 |
| MOTA | 11681 | CG | LYS | 1731 | 25.726 | -4.683 -19.587 | 1.00 29.75 |
| ATOM | 11682 | CD | LYS | 1731 | 26.304 | -5.843 -20.375 | 1.00 31.89 |
| ATOM | 11683 | CE | LYS | 1731. | | -6.072 -21.667 | 1.00 32.08 |
| ATOM | 11684 | NZ | LYS | 1731 | 26.136 | -7.215 -22.417 | 1.00 34.11 |
| ATOM | 11685 | C | LYS | 1731 | 24.431 | -3.361 -17.307 | 1.00 25.48 |
| ATOM | 11686 | o | LYS | 1731 | 23.868 | -4.094 -16.498 | 1.00 24.67 |
| | | | | | 23.779 | -2.534 -18.113 | 1.00 24.62 |
| ATOM | 11687 | N | ASN | 1732 | | -2.450 -18.112 | |
| АТОМ | 11688 | CA | ASN | 1732 | 22.326 | | 1.00 24.54 |
| ATOM | 11689 | CB | ASN | 1732 | 21.883 | -1.055 -18.565 | 1.00 23.33 |
| ATOM | 11690 | CG | ASN | 1732 | 20.371 | -0.911 -18.640 | 1.00 21.61 |
| ATOM | 11691 | OD1 | ASN | 1732 | 19.637 | -1.889 -18.565 | 1.00 19.03 |
| MOTA | 11692 | ND2 | ASN | 1732 | 19.903 | 0.326 -18.804 | 1.00 23.82 |
| ATOM | 11693 | С | ASN | 1732 | 21.785 | -3.508 -19.068 | 1.00 25.76 |
| MOTA | 11694 | 0 | ASN | 1732 | 21.773 | -3.302 -20.283 | 1.00 25.61 |
| ATOM | 11695 | N | PHE | 1733 | 21.344 | -4.637 -18.520 | 1.00 25.01 |
| ATOM | 11696 | CA | PHE | 1733 | 20.811 | -5.719 -19.337 | 1.00 25.29 |
| ATOM | 11697 | CB | PHE | 1733 | 20.880 | -7.049 -18.582 | 1.00 26.19 |
| MOTA | 11698 | CG | PHE | 1733 | 22.279 | -7.524 -18.325 | 1.00 25.90 |
| | | | PHE | 1733 | 22.973 | -7.108 -17.195 | 1.00 26.87 |
| MOTA | 11699 | | | | | | 1.00 26.66 |
| MOTA | 11700 | | PHE | 1733 | 22.922 | | |
| ATOM | 11701 | | PHE | 1733 | 24.292 | -7.510 -16.975 | 1.00 25.54 |
| MOTA | 11702 | CE2 | PHE | 1733 | 24.242 | -8.761 -19.029 | 1.00 26.56 |
| MOTA | 11703 | cz | PHE | 1733 | 24.926 | -8.335 -17.895 | 1.00 27.21 |
| MOTA | 11704 | C. | PHE | 1733 - | | -5.471 -19.807 | 1.00 26.55 |
| MOTA | 11705 | 0 | PHE | 1733 | 18.902 | -6.133 -20.726 | 1.00 22.93 |
| MOTA | 11706 | N | LEU | 1734 | 18.696 | -4.521 -19.178 | 1.00 27.50 |
| ATOM | 11707 | CA | LEU | 1734 | 17.330 | -4.212 -19.569 | 1.00 29.76 |
| MOTA | 11708 | CB | LEU | 1734 | 16.605 | -3.451 -18.461 | 1.00 28.65 |
| ATOM | 11709 | CG | LEU | 1734 | 15.196 | -2.972 -18.829 | 1.00 27.48 |
| ATOM | 11710 | | LEU | 1734 | 14.348 | -4.147 -19.304 | 1.00 25.62 |
| ATOM | 11711 | | LEU | 1734 | 14.566 | -2.305 -17.625 | 1.00 23.90 |
| ATOM | 11712 | C | LEU | 1734 | 17.293 | -3.383 -20.847 | 1.00 32.37 |
| ATOM | 11713 | 0 | LEU | 1734 | 16.613 | -3.748 -21.804 | 1.00 31.12 |
| | | | | | 18.023 | -2.270 -20.855 | 1.00 36.48 |
| ATOM | 11714 | N | ALA | 1735 | | | |
| ATOM | 11715 | CA | ALA | 1735 | 18.068 | -1.378 -22.011 | 1.00 42.29 |
| ATOM | 11716 | СВ | ALA | 1735 | 19.293 | -0.470 -21.929 | 1.00 42.69 |
| MOTA | 11717 | С | ALA | 1735 | 18.100 | -2.186 -23.297 | 1.00 46.05 |
| MOTA | 11718 | 0 | ALA | 1735 | 17.499 | -1.801 -24.307 | 1.00 46.72 |
| MOTA | 11719 | N | GLU | 1736 | 18.797 | -3.317 -23.239 | 1.00 49.05 |
| ATOM | 11720 | CA | GLU | 1736 | 18.923 | -4.225 -24.374 | 1.00 51.86 |
| MOTA | 11721 | CB | GLU | 1736 | 19.548 | -5.551 -23.913 | 1.00 53.55 |
| ATOM | 11722 | CG | GLU | 1736 | 20.814 | -5.411 -23.072 | 1.00 55.23 |
| ATOM | 11723 | CD | GLU | 1736 | 22.018 | -4.944 -23.873 | 1.00 57.29 |
| ATOM | 11724 | | GLU | 1736 | 21.940 | -3.866 -24.505 | 1.00 58.69 |
| ATOM | 11725 | OE2 | | 1736 | 23.046 | -5.657 -23.869 | 1.00 57.04 |
| ATOM | 11726 | C | GLU | 1736 | 17.546 | -4.495 -24.986 | 1.00 57.04 |
| | | | | | | -4.351 -26.195 | 1.00 53.04 |
| ATOM | 11727 | 0 | GLU | 1736 | 17.355 | | |
| ATOM | 11728 | N | THR | 1737 | 16.594 | -4.876 -24.134 | 1.00 51.41 |
| MOTA | 11729 | CA | THR | 1737 | 15.228 | -5.187 -24.551 | 1.00 49.15 |
| ATOM | 11730 | CB | THR | 1737 | 14.969 | -6.699 -24.442 | 1.00 50.52 |
| MOTA | 11731 | | THR | 1737 | 13.658 | -7.002 -24.935 | 1.00 54.05 |
| MOTA | 11732 | CG2 | THR | 1737 | 15.082 | -7.146 -22.993 | 1.00 51.48 |
| | | | | | | | |

| MOTA | 11733 | С | THR | 1737 | | 14.202 | -4.449 | -23.685 | 1.00 46.27 |
|-------|-------|-----|-----|-------|-----|--------|---------|---------|------------|
| MOTA | 11734 | 0 | THR | 1737 | | 14.491 | -3.381 | -23.149 | 1.00 47.44 |
| ATOM | 11735 | N | GLY | 1738 | | 13.004 | -5.015 | -23.557 | 1.00 42.24 |
| MOTA | 11736 | CA | GLY | 1738 | | 11.969 | | -22.742 | 1.00 36.72 |
| ATOM | 11737 | C | GLY | 1738 | | 11.296 | | -21.831 | 1.00 33.77 |
| | | | | | | 10.106 | | -21.520 | 1.00 31.85 |
| MOTA | 11738 | 0 | GLY | 1738 | | | | | |
| MOTA | 11739 | N | ASP | 1739 | | 12.076 | | -21.398 | 1.00 31.02 |
| ATOM | 11740 | CA | ASP | 1739 | | 11.587 | | -20.535 | 1.00 29.23 |
| MOTA | 11741 | CB | ASP | 1739 | | 11.418 | | -21.358 | 1.00 32.58 |
| MOTA | 11742 | CG | ASP | 1739 | | 10.678 | -9.832 | -20.609 | 1.00 35.23 |
| ATOM | 11743 | OD1 | ASP | 1739 | | 11.103 | -10.195 | -19.493 | 1.00 35.59 |
| MOTA | 11744 | OD2 | ASP | 1739 | | 9.667 | -10.332 | -21.147 | 1.00 38.35 |
| ATOM | 11745 | Ć | ASP | 1739 | | 12.612 | -7.688 | -19.425 | 1.00 26.10 |
| ATOM | 11746 | 0 | ASP | 1739 | | 13.748 | | -19.691 | 1.00 24.19 |
| ATOM | 11747 | N | ILE | 1740 | | 12.215 | | -18.184 | 1.00 23.09 |
| | 11748 | CA | ILE | 1740 | | 13.111 | | -17.050 | 1.00 21.06 |
| MOTA | | | | | | 12.454 | | -15.740 | 1.00 20.26 |
| MOTA | 11749 | CB | ILE | 1740 | | | | | |
| MOTA | 11750 | CG2 | | 1740 | | 13.307 | | -14.531 | 1.00 21.30 |
| MOTA | 11751 | | ILE | 1740 | | 12.300 | | -15.794 | 1.00 20.28 |
| MOTA | 11752 | CD1 | ILE | 1740 | | 11.517 | | -14.637 | 1.00 21.21 |
| MOTA | 11753 | С | ILE | 1740 | | 13.545 | -9.049 | -16.896 | 1.00 19.53 |
| MOTA | 11754 | 0 | ILE | 1740 | | 14.724 | -9.337 | -16.663 | 1.00 20.00 |
| ATOM | 11755 | N | ARG | 1741 | | 12.600 | -9.971 | -17.030 | 1.00 18.98 |
| ATOM | 11756 | CA | ARG | 1741 | | 12.937 | -11.384 | -16.911 | 1.00 19.96 |
| ATOM | 11757 | CB | ARG | 1741 | | | -12.236 | | 1.00 19.87 |
| ATOM | 11758 | CG | ARG | 1741 | | | -12.142 | | 1.00 21.32 |
| | | CD | ARG | 1741 | | | -12.853 | | 1.00 23.47 |
| ATOM | 11759 | | | | | | | | 1.00 25.47 |
| ATOM | 11760 | NE | ARG | 1741 | | | -12.794 | | |
| ATOM | 11761 | CZ | ARG | 1741 | | | -11.676 | | 1.00 27.35 |
| MOTA | 11762 | | ARG | 1741 | | | -10.514 | | 1.00 29.85 |
| MOTA | 11763 | | ARG | 1741 | | | -11.716 | | 1.00 28.28 |
| ATOM | 11764 | С | ARG | 1741 | | 13.936 | -11.809 | -17.984 | 1.00 20 67 |
| MOTA | 11765 | 0 | ARG | 1741 | | 14.888 | -12.546 | -17.702 | 1.00 20.44 |
| ATOM | 11766 | N | ALA | 1742 | | 13.733 | -11.333 | -19.209 | 1.00 18.88 |
| ATOM | 11767 | CA | ALA | 1742 | | 14.642 | -11.663 | -20.299 | 1.00 19.67 |
| ATOM | 11768 | СВ | ALA | 1742 | | | -11.119 | | 1.00 17.58 |
| ATOM | 11769 | C | ALA | 1742 | | | -11.057 | | 1.00 19.77 |
| ATOM | 11770 | Ö | ALA | 1742 | | | -11.601 | | 1.00 21.64 |
| | | | | | | 16.011 | | -19.308 | 1.00 19.15 |
| ATOM | 11771 | N | ALA | 1743 | | | | | |
| ATOM | 11772 | CA | ALA | 1743 | | 17.245 | | -18.946 | 1.00 18.94 |
| MOTA | 11773 | CB | ALA | 1743 | | 16.934 | | -18.354 | 1.00 19.04 |
| MOTA | 11774 | С | ALA | 1743 | | | -10.095 | | 1.00 19.62 |
| MOTA | 11775 | 0 | ALA | 1743 | | 19.231 | -10.194 | -17.984 | 1.00 19.37 |
| MOTA | 11776 | N | VAL | 17.44 | | 17.268 | -10.706 | -17.010 | 1.00 20.08 |
| MOTA | 11777 | CA | VAL | 1744 | | 17.861 | -11.560 | -15.992 | 1.00 19.96 |
| ATOM | 11778 | CB | VAL | 1744 | | 16.791 | -12.000 | -14.961 | 1.00 21.45 |
| ATOM | 11779 | | | | . % | | -13.143 | | 1.00 19.83 |
| ATOM | 11780 | | VAL | 1744 | | | -10.812 | | 1.00 18.35 |
| ATOM | 11781 | C | VAL | 1744 | | | -12.783 | | 1.00 22.05 |
| | 11782 | 0 | VAL | 1744 | | | -13.197 | | 1.00 21.12 |
| ATOM | | | | | | | -13.356 | | 1.00 21.99 |
| ATOM | 11783 | N | ARG | 1745 | | | | | |
| ATOM | 11784 | CA | ARG | 1745 | | | -14.515 | | 1.00 24.40 |
| ATOM | 11785 | CB | ARG | 1745 | | | -15.066 | | 1.00 25.74 |
| ATOM | 11786 | CG | ARG | 1745 | | | -15.664 | | 1.00 26.03 |
| ATOM | 11787 | CD | ARG | 1745 | | 15.141 | | -19.527 | 1.00 29.74 |
| ATOM | 11788 | NE | ARG | 1745 | | | -15.629 | -20.580 | 1.00 31.09 |
| ATOM | 11789 | cz | ARG | 1745 | | | -14.924 | | 1.00 33.26 |
| ATOM | 11790 | NH1 | ARG | 1745 | | 12.767 | -14.957 | -19.320 | 1.00 31.03 |
| ATOM | 11791 | NH2 | ARG | 1745 | | 13.024 | -14.183 | -21.470 | 1.00 33.72 |
| ATOM | 11792 | С | ARG | 1745 | | 19.523 | -14.161 | -19.126 | 1.00 24.45 |
| ATOM | 11793 | 0 - | ARG | 1745 | | 20.420 | -14.994 | | 1.00 23.74 |
| ATOM | 11794 | N | GLN | 1746 | | | -12.925 | | 1.00 24.53 |
| | | | | | | | -12.490 | | 1.00 24.66 |
| ATOM | 11795 | CA | GLN | 1746 | | | -11.120 | | 1.00 24.00 |
| ATOM | 11796 | CB | GLN | 1746 | | | | | |
| ATOM | 11797 | CG | GLN | 1746 | | | -10.729 | | 1.00 26.46 |
| ATOM | 11798 | CD | GLN | 1746 | | 21.249 | | -22.651 | 1.00 28.72 |
| ATOM | 11799 | | GLN | 1746 | | 20.132 | -9.019 | | 1.00 27.11 |
| ATOM | 11800 | NE2 | GLN | 1746 | | 22.282 | | -22.662 | 1.00 30.62 |
| MOTA | 11801 | С | GLN | 1746 | | 21.984 | -12.410 | -19.491 | 1.00 24.23 |
| ATOM | 11802 | 0 | GLN | 1746 | | 23.071 | -12.850 | -19.860 | 1.00 23.92 |
| MOTA | 11803 | N | TYR | 1747 | | 21.800 | -11.831 | -18.311 | 1.00 23.27 |
| ATOM | 11804 | CA | TYR | 1747 | | 22.883 | -11.693 | -17.352 | 1.00 22.18 |
| ATOM | 11805 | СВ | TYR | 1747 | | 22.363 | -10.949 | | 1.00 21.72 |
| ATOM | 11806 | CG | TYR | 1747 | | | -10.978 | | 1.00 20.80 |
| ATOM | | | | 1747 | | | -10.575 | | 1.00 20.83 |
| | 11807 | CD1 | | | | | | | 1.00 20.83 |
| ATOM. | 11808 | CE1 | | 1747 | | | -10.540 | | |
| MOTA | 11809 | CD2 | TYR | 1747 | | 22.194 | -11.446 | -13.0// | 1.00 20.71 |

```
ATOM 11810 CE2 TYR 1747
                                 23.610 -11.463 -12.546 1.00 21.91
ATOM
     11811 CZ
                 TYR
                       1747
                                 24.913 -11.011 -12.640
                                                          1.00 20.88
                                 25.730 -11.044 -11.530
                                                          1.00 22.08
MOTA
      11812
             OH
                 TYR
                       1747
                       1747
                                 23.417 -13.079 -16.987
                                                          1.00 21.20
ATOM
      11813
             С
                  TYR
                       1747
                                 24.625 -13.303 -16.992
MOTA
      11814
             0
                 TYR
                                                          1.00 21.41
      11815
                 MET
                       1748
                                 22.516 -14.010 -16.692
                                                          1.00 19.89
MOTA
             N
                       1748
                                 22.915 -15.370 -16.327
                                                          1.00 22.82
ATOM
      11816
             CA
                 MET
                                 21.680 -16.205 -15.994
             CB
                 MET
                       1748
                                                          1.00 22.86
ATOM
      11817
                                 20.883 -15.673 -14.814
                                                          1.00 24.78
MOTA
      11818
             CG
                 MET
                       1748
                                 19.282 -16.477 -14.671
      11819
             SD
                 MET
                       1748
                                                          1.00 29.17
MOTA
                 MET
                       1748
                                 19.786 -18.014 -13.979
                                                          1.00 26.45
MOTA
      11820
             CE
                                 23.692 -16.047 -17.452
                 MET
                       1748
                                                          1.00 22.62
ATOM
      11821
             С
                                 24.653 -16.786 -17.213
                                                          1.00 21.81
      11822
                 MET
                       1748
ATOM
             0
                                 23.262 -15.790 -18.680
                                                          1.00 22.35
MOTA
      11823
             N
                 ALA
                       1749
                       1749
                                 23.900 -16.374 -19.848
                                                          1.00 21.37
ATOM
      11824
             CA
                 ALA
                                 22.980 -16.228 -21.061
                                                          1.00 22.11
MOTA
      11825
             CB
                 ALA
                       1749
                 ALA
                       1749
                                 25.268 -15.766 -20.148
                                                          1.00 20.89
ATOM
      11826
             С
                                 26.212 -16.489 -20.461
                                                          1.00 23.24
ATOM
      11827
             0
                 ALA
                       1749
                                 25.390 -14.446 -20.053
MOTA
      11828
             N
                 GLU
                       1750
                                                          1.00 21.41
                                 26.671 -13.808 -20.352
MOTA
      11829
             CA
                 GLU
                       1750
                                                          1.00 21.76
             CB
                       1750
                                 26.497 -12.300 -20.528
                                                          1.00 23.39
ATOM
      11830
                 GLU
                                 25.501 -11.917 -21.613
                                                          1.00 25.73
                       1750
                 GLU
ATOM
      11831
             CG
                                 25.685 -10.499 -22.093
                                                          1.00 25.79
ATOM
      11832
             CD
                 GLU
                       1750
                                 26.438 -9.746 -21.442
MOTA
      11833
             OE1
                 GLU
                       1750
                                                          1.00 25.87
                                 25.070 -10.130 -23.123
                                                          1.00 28.21
MOTA
      11834
             OE2 GLU
                       1750
                                 27.749 -14.084 -19.307
                                                          1.00 23.50
MOTA
      11835
                 GLU
                       1750
             C
                                 28.942 -14.115 -19.627
                                                          1.00 21.76
ATOM
      11836
             0 .
                 GLU
                       1750
ATOM
      11837
                 VAL
                       1751
                                 27.345 -14.269 -18.054
                                                          1.00 23.02
             N
MOTA
      11838
             CA
                 VAL
                       175İ
                                 28.317 -14.558 -17.007
                                                          1.00 23.63
                                 27.674 -14.482 -15.593
                       1751
                                                          1.00 23.59
ATOM
      11839
             CB
                 VAL
                                                          1.00 22.90
                                 28.597 -15.124 -14.563
MOTA
      11840
             CG1 VAI
                       1751
                                 27.431 -13.029 -15.214 1.00 22.54
MOTA
      11841
             CG2
                 VAL
                       1751
                       1751
                                 28.893 -15.952 -17.233
                                                          1.00 24.14
MOTA
      11842
             С
                 VAL
                                                          1.00 25.38
                                 30.100 -16.164 -17.100
MOTA
      11843
             0
                 VAL
                       1751
                                 28.028 -16.895 -17.589
                                                          1.00 24.05
ATOM
      11844
                 GLU
                       1752
             N
                                 28.459 -18.264 -17.834
                                                          1.00 26.81
ATOM
      11845
             CA
                 GLU
                       1752
                                 27.247 -19.196 -17.907
                                                          1.00 28.09
MOTA
      11846
             CB.
                 GLU
                       1752
                       1752
                                 27.611 -20.655 -18.151
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MOTA
      11847
             CG
                 GLU
                                 26.452 -21.589 -17.904
MOTA
      11848
             CD
                 GLU
                       1752
                                                          1.00 30.97
                                 26.551 -22.775 -18.279
                                                          1.00 32.52
ATOM
      11849
             OE1 GLU
                       1752
                                 25.439 -21.143 -17.328
29.284 -18.397 -19.113
                                                          1.00 31.48
MOTA
      11850
             OE2 GLU
                       1752
MOTA
      11851
                 GLU
                       1752
                                                          1.00 28.55
             С
                                                          1.00 29.30
ATOM
      11852
             0
                 GLU
                       1752
                                 30.237 -19.173 -19.164
                 SER
                       1753
                                 28.914 -17.646 -20.146
                                                          1.00 28.43
ATOM
      11853
             N
                                 29.640 -17.701 -21.413
                                                          1.00 29.68
                       1753
                 SER
ATOM
      11854
             CA
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      11855
             CB
                 SER
                       1753
MOTA
                       1753
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             OG
                 SER
                       1753
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                 SER
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                       1753
             O
                                 31.047 -16.013 -20.404
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                       1754
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ATOM
      11860
            CA
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                       1754
                                                          1.00 27.36
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                       1754
                                                          1.00 26.65
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      11861
             С
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ATOM
      11862 O
                 GLY
                      1754
                                                          1.00 26.59
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1.00 26.68
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ATOM
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            N
ATOM
      11864
             CA
                 VAL
                       1755
                       1755
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             CG1
                 VAL
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             CG2 VAL
                      1755
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ATOM
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ATOM
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             С
                 VAL
                                                          1.00 25.55
ATOM
      11869
            .0
                 VAL
                       1755
      11870
                       1756
                                 30.346 -11.480 -20.068
                                                          1.00 25.63
ATOM
            N
                 TYR
                                                          1.00 25.13
ATOM
      11871
             CA
                 TYR
                       1756
                                 30.233 -10.455 -19.031
                                 28.764 -10.150 -18.707
                                                          1.00 25.56
                       1756
ATOM
      11872
             CB
                 TYR
                                 28.618 -9.068 -17.657
                                                          1.00 24.46
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      11873
             CG
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                       1756
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ATOM
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                       1756
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                                 28.319
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                 TYR
MOTA
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                 TYR
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      11880
                 TYR
                       1756
             С
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                 TYR
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                 PRO
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ATOM
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             CD
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ATOM
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             CA
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ATOM
      11885
             CB
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ATOM
      11886
                 PRO
                       1757
                                 33.281 -9.082 -15.679
                                                         1.00 29.30
             CG
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| MOTA | 11887 | С | PRO | 1757 | 33.031 | -8.664 | -18.761 | 1.00 30.41 |
|--------------|----------------|----------|------------|------|--------|--------------------|---------|------------|
| ATOM | 11888 | 0 | PRO | 1757 | 33.900 | -9.529 | -18.855 | 1.00 30.25 |
| ATOM | 11889 | N | GLY | 1758 | 32.911 | -7.663 | -19.627 | 1.00 31.45 |
| MOTA | 11890 | CA | GLY | 1758 | 33.839 | -7.537 | -20.735 | 1.00 32.26 |
| ATOM | 11891 | С | GLY | 1758 | 35.007 | -6.657 | -20.339 | 1.00 33.47 |
| ATOM | 11892 | 0 | GLY | 1758 | 35.073 | -6.183 | -19.202 | 1.00 30.45 |
| ATOM | 11893 | N | GLU | 1759 | 35.932 | -6.427 | -21.265 | 1.00 34.20 |
| MOTA | 11894 | CA | GLU | 1759 | 37.088 | -5.589 | -20.966 | 1.00 36.05 |
| MOTA | 11895 | CB | GLU | 1759 | 38.020 | -5.500 | -22.179 | 1.00 37.61 |
| MOTA | 11896 | CG | GLU | 1759 | 39.230 | -4.611 | -21.932 | 1.00 39.60 |
| MOTA | 11897 | CD | GLU | 1759 | 40.075 | -5.093 | -20.765 | 1.00 40.84 |
| ATOM | 11898 | OE1 | GLU | 1759 | 40.868 | -4.288 | -20.231 | 1.00 43.08 |
| ATOM | 11899 | OE2 | GLU | 1759 | 39.949 | -6.278 | -20.390 | 1.00 40.65 |
| ATOM | 11900 | С | GLU | 1759 | 36.665 | -4.181 | -20.550 | 1.00 36.19 |
| MOTA | 11901 | 0 | GLU | 1759 | 37.293 | -3.560 | -19.693 | 1.00 36.76 |
| MOTA | 11902 | N | GLU | 1760 | 35.596 | -3.683 | -21.162 | 1.00 37.70 |
| ATOM | 11903 | CA | GLU | 1760 | 35.095 | -2.347 | -20.863 | 1.00 38.57 |
| ATOM | 11904 | CB | GLU | 1760 | 33.950 | -1.980 | -21.809 | 1.00 41.14 |
| ATOM | 11905 | CG | GLU | 1760 | 34.038 | -2.619 | -23.182 | 1.00 43.82 |
| MOTA | 11906 | CD | GLU | 1760 | 33.669 | -4.089 | -23.154 | 1.00 44.67 |
| ATOM | 11907 | OE1 | GLU | 1760 | 32.538 | -4.404 | -22.730 | 1.00 45.33 |
| ATOM | 11908 | OE2 | GLU | 1760 | 34.508 | -4.925 | -23.556 | 1.00 45.49 |
| ATOM | 11909 | C | GLU | 1760 | 34.598 | -2.255 | -19.426 | 1.00 37.43 |
| ATOM | 11910 | 0 | GLU | 1760 | 34.479 | -1.162 | -18.873 | 1.00 37.27 |
| ATOM | 11911 | N | HIS | 1761 | 34.306 | -3.411 | -18.835 | 1.00 36.62 |
| ATOM | 11912 | CA | HIS | 1761 | 33.809 | -3.487 | -17.462 | 1.00 36.41 |
| ATOM | 11913 | CB | HIS | 1761 | 32.650 | | -17.373 | 1.00 34.33 |
| MOTA | 11914 | CG | HIS | 1761 | 31.541 | | -18.343 | 1.00 33.22 |
| ATOM | 11915 | | HIS | 1761 | 31.033 | | -19.346 | 1.00 31.29 |
| ATOM | 11916 | ND1 | HIS | 1761 | 30.806 | -3.053 | -18.329 | 1.00 32.96 |
| ATOM | 11917 | | HIS | 1761 | 29.892 | | -19.281 | 1.00 32.22 |
| ATOM | 11918 | | HIS | 1761 | 30.008 | | -19.912 | 1.00 32.69 |
| ATOM | 11919 | C | HIS | 1761 | 34.905 | | -16.504 | 1.00 37.42 |
| ATOM | 11920 | ō | HIS | 1761 | 34.620 | | -15.369 | 1.00 38.41 |
| ATOM | 11921 | N | SER | 1762 | 36.153 | | -16.960 | 1.00 37.25 |
| ATOM | 11922 | CA | SER | 1762 | 37.276 | | -16.144 | 1.00 37.81 |
| ATOM | 11923 | СВ | SER | 1762 | 37.960 | | -16.819 | 1.00 37.82 |
| ATOM | 11924 | OG | SER | 1762 | 37.022 | | -17.142 | 1.00 36.90 |
| ATOM | 11925 | C | SER | 1762 | 38.309 | | -15.884 | 1.00 39.62 |
| ATOM | 11926 | ō | SER | 1762 | 38.410 | | -16.642 | 1.00 37.84 |
| ATOM | 11927 | N | PHE | 1763 | 39.069 | | -14.802 | 1.00 40.54 |
| MOTA | 11928 | CA | PHE | 1763 | 40.112 | | -14.458 | 1.00 43.38 |
| MOTA | 11929 | CB | PHE | 1763 | 39.929 | | -13.037 | 1.00 44.18 |
| ATOM | 11930 | CG | PHE | 1763 | 38.661 | | -12.840 | 1.00 45.64 |
| ATOM | 11931 | | PHE | 1763 | 37.477 | | -12.485 | 1.00 46.71 |
| ATOM | 11932 | | PHE | 1763 | 38.648 | | -13.014 | 1.00 46.22 |
| ATOM | 11933 | | PHE | 1763 | 36.297 | | -12.305 | 1.00 46.58 |
| ATOM | 11934 | CE2 | | 1763 | 37.475 | | -12.838 | 1.00 46.28 |
| ATOM | 11935 | CZ | PHE | 1763 | 36.297 | | -12.482 | 1.00 46.49 |
| ATOM | 11936 | C | PHE | 1763 | 41.475 | | -14.567 | 1.00 45.31 |
| ATOM | 11937 | ō | PHE | 1763 | 41.568 | | -14.742 | 1.00 45.15 |
| ATOM | 11938 | N | | 1764 | 42.531 | | | 1.00 47.11 |
| ATOM | 11939 | CA | HIS | 1764 | 43.897 | | -14.551 | 1.00 48.73 |
| ATOM | 11940 | CB | HIS | 1764 | 44.368 | | -16.007 | 1.00 48.11 |
| ATOM | 11941 | CG | HIS | 1764 | 43.714 | | -16.858 | 1.00 47.92 |
| ATOM | 11942 | | HIS | 1764 | 42.833 | | -17.881 | 1.00 47.14 |
| ATOM | 11943 | | HIS | 1764 | 43.935 | | -16.681 | 1.00 48.69 |
| ATOM | 11944 | | HIS | 1764 | 43.218 | | -17.557 | 1.00 47.18 |
| ATOM | 11945 | | HIS | 1764 | 42.541 | | -18.297 | 1.00 46.67 |
| ATOM | 11946 | C | HIS | 1764 | 44.848 | | -13.694 | 1.00 49.73 |
| ATOM | 11947 | ō | HIS | 1764 | 45.534 | | -12.839 | 1.00 50.49 |
| ATOM | 11948 | | HIS | 1764 | 44.896 | | -13.887 | 1.00 51.77 |
| ATOM | 11949 | C1 | KPL | 1765 | 27.748 | -4.209 | -4.469 | 1.00 37.13 |
| MOTA | 11949 | C2 | KPL | 1765 | 27.740 | -5.559 | -3.746 | 1.00 37.13 |
| ATOM | 11951 | C3 | KPL | 1765 | 27.104 | -6.630 | -4.447 | 1.00 36.77 |
| ATOM | 11952 | C4 | KPL | 1765 | 29.432 | -5.968 | -3.834 | 1.00 38.31 |
| ATOM | 11953 | 01 | KPL | 1765 | 30.255 | -4.985 | -3.190 | 1.00 40.50 |
| ATOM | 11954 | C5 | KPL | 1765 | 27.511 | -5.432 | -2.265 | 1.00 40.30 |
| ATOM | 11954 | 02 | KPL | 1765 | 28.306 | -5.650 | -1.372 | 1.00 36.08 |
| | | C6 | | 1765 | 26.106 | -5.037 | -1.885 | 1.00 33.38 |
| ATOM ATOM | 11956 11957 | 03 | KPL KPL | 1765 | 25.273 | -4.814 | -2.736 | 1.00 35.38 |
| | 11957 | | | 1765 | 25.770 | -4.927 | -0.590 | 1.00 33.07 |
| MOTA | | 04 CB | KPL | | 10.432 | -42.440 | 39.264 | 1.00 32.90 |
| ATOM | 11959 | CB | MET | 1801 | | | 39.475 | 1.00 62.99 |
| ATOM | 11960 | CG | MET | 1801 | 11.787 | -41.787 | 40.338 | 1.00 64.83 |
| ATOM | 11961 | SD | MET | 1801 | | -42.311 | 40.338 | 1.00 67.79 |
| ATOM | 11962 | CE | MET | 1801 | | -42.311 -40.780 | 40.307 | 1.00 67.34 |
| MOTA | 11963 | С | MET | 1801 | 0.031 | -0.700 | 30.307 | 1.00 39.13 |

| ATOM | 11964 | 0 | MET | 1801 | 7.710 | -40.737 | 40.655 | 1.00 59.38 |
|--------------|----------------|----------|------------|--------------|--------|--------------------|------------------|--------------------------|
| ATOM | 11965 | N | MET | 1801 | | -40.456 | 37.968 | 1.00 61.53 |
| ATOM | 11966 | CA | MET | 1801 | | -41.449 | 38.998 | 1.00 60.88 |
| ATOM | 11967 | N | LYS | 1802 | | -40.256 | 41.033 | 1.00 56.22 |
| ATOM | 11968 | CA | LYS | 1802 | | -39.612 | 42.312 | 1.00 53.19 |
| ATOM | 11969 | СВ | LYS | 1802 | | -40.624 | 43.447 | 1.00 54.60 |
| ATOM | 11970 | CG | LYS | 1802 | | -41.941 | 43.283 | 1.00 55.72 |
| ATOM | 11971 | CD | LYS | 1802 | | -41.813 | 43.598 | 1.00 56.31 |
| ATOM | 11972 | CE | LYS | 1802 | | -41.678 | 45.099 | 1.00 56.54 |
| | 11972 | NZ | LYS | 1802 | | -41.687 | 45.436 | 1.00 55.62 |
| ATOM | 11973 | | | 1802 | | -38.361 | 42.596 | 1.00 49.88 |
| ATOM | | C | LYS | | | -38.088 | 43.759 | 1.00 50.44 |
| ATOM | 11975 | 0 | LYS | 1802 | | -37.590 | 41.560 | 1.00 30.44 |
| ATOM | 11976 | N | PRO | 1803 | | | 41.816 | 1.00 43.32 |
| ATOM | 11977 | CD | PRO | 1803 | | -36.225 | 40.132 | 1.00 41.04 |
| ATOM | 11978 | CA | PRO | 1803 | | -37.761 | | 1.00 41.04 |
| ATOM | 11979 | CB | PRO | 1803 | | -36.334 | 39.651 | |
| MOTA | 11980 | CG | PRO | 1803 | | -35.650 | 40.414 | 1.00 43.86 |
| ATOM | 11981 | С | PRO | 1803 | | -38.481 | 39.414 | 1.00 36.05 |
| ATOM | 11982 | 0 | PRO | 1803 | | -38.991 | 40.056 | 1.00 34.80 |
| ATOM | 11983 | N | THR | 1804 | | -38.511 | 38.084 | 1.00 30.62 |
| MOTA | 11984 | CA | THR | 1804 | | -39.155 | 37.283 | 1.00 26.97 |
| MOTA | 11985 | CB | THR | 1804 | | -39.435 | 35.853 | 1.00 25.88 |
| ATOM | 11986 | | THR | 1804 | | -40.323 | 35.902 | 1.00 24.56 |
| MOTA | 11987 | | THR | 1804 | | -40.073 | 35.021 | 1.00 22.12 |
| MOTA | 11988 | C | THR | 1804 | | -38.232 | 37.215 | 1.00 24.43 |
| ATOM | 11989 | 0 | THR | 1804 | | -37.056 | 36.888 | 1.00 22.49 |
| MOTA | 11990 | N | THR | 1805 | | -38.769 | 37.524 | 1.00 23.84 |
| MOTA | 11991 | CA | THR | 1805 | 16.278 | -37.973 | 37.516 | 1.00 22.21 |
| ATOM | 11992 | CB | THR | 1805 | | -37.800 | 38.940 | 1.00 23.39 |
| ATOM | 11993 | OG1 | | 1805 | | -39.072 | 39.423 | 1.00 25.01 |
| MOTA | 11994 | CG2 | THR | 1805 | | -37.267 | 39.866 | 1.00 23.36 |
| ATOM | 11995 | C | THR | 1805 | | -38.614 | 36.682 | 1.00 21.44 |
| ATOM | 11996 | 0 | THR | 1805 | | -39.761 | 36.247 | 1.00 19.91 1.00 19.22 |
| ATOM | 11997 | N | ILE | 1806 | | -37.863 | 36.471 | 1.00 19.22 |
| ATOM | 11998 | CA | ILE | 1806 | | -38.376 | 35.706 | 1.00 20.33 |
| MOTA | 11999 | CB | ILE | 1806 | | -37.329 -37.846 | 35.599 34.689 | 1.00 22.61 |
| MOTA | 12000 | CG2 | | 1806 | | -36.030 | 35.016 | 1.00 23.30 |
| MOTA | 12001 | CG1 | | 1806 | | -34.859 | 35.129 | 1.00 24.71 |
| MOTA | 12002 | CD1 C | ILE ILE | 1806 1806 | 20.108 | -39.623 | 36.415 | 1.00 27.80 |
| ATOM ATOM | 12003 12004 | 0 | ILE | 1806 | 20.100 | -40.551 | 35.780 | 1.00 17.26 |
| ATOM | 12005 | N | SER | 1807 | | -39.652 | 37.736 | 1.00 19.88 |
| MOTA | 12006 | CA | SER | 1807 | 20.455 | -40.796 | 38.505 | 1.00 20.30 |
| MOTA | 12007 | CB | SER | 1807 | | -40.578 | 40.000 | 1.00 22.82 |
| ATOM | 12008 | OG | SER | 1807 | 20.872 | -39.418 | 40.459 | 1.00 29.05 |
| ATOM | 12009 | C | SER | 1807 | 19.777 | -42.090 | 38.062 | 1.00 19.29 |
| ATOM | 12010 | ō | SER | 1807 | | -43.148 | 38.010 | 1.00 18.78 |
| ATOM | 12011 | N | LEU | 1808 | | -42.002 | 37.741 | 1.00 19.36 |
| ATOM | 12012 | CA | LEU | 1808 | 17.731 | -43.170 | 37.317 | 1.00 19.70 |
| ATOM | 12013 | CB | LEU | 1808 | 16.248 | -42.828 | 37.204 | 1.00 21.62 |
| MOTA | 12014 | CG | LEU | 1808 | 15.233 | -43.791 | 37.821 | 1.00 26.64 |
| MOTA | 12015 | | LEU | 1808 | 13.896 | -43.565 | 37.130 | 1.00 27.41 |
| ATOM | 12016 | CD2 | LEU | 1808 | 15.658 | -45.247 | 37.649 | 1.00 26.23 |
| MOTA | 12017 | C | LEU | 1808 | 18.218 | -43.719 | 35.984 | 1.00 17.67 |
| MOTA | 12018 | 0 | LEU | 1808 | 18.294 | -44.934 | 35.797 | 1.00 16.92 |
| MOTA | 12019 | N | LEU | 1809 | 18.528 | -42.831 | 35.047 | 1.00 16.05 |
| MOTA, | 12020 | CA | LEU | 1809 | | -43.273 | 33.740 | 1.00 15.75 |
| MOTA | 12021 | CB | LEU | 1809 | | -42.089 | 32.772 | |
| MOTA | 12022 | CG | LEU | 1809 | | -41.302 | 32.527 | 1.00 16.26 |
| MOTA | 12023 | CD1 | LEU | 1809 | 18.026 | -40.320 | 31.380 | 1.00 11.13 |
| MOTA | 12024 | CD2 | LEU | 1809 | | -42.238 | 32.202 | 1.00 15.56 |
| MOTA | 12025 | С | LEU | 1809 | | -43.936 | 33.900 | 1.00 16.76 |
| MOTA | 12026 | 0 | LEU | 1809 | | -44.952 | 33.267 | 1.00 17.33 |
| MOTA | 12027 | N | GLN | 1810 | | -43.363 | 34.752 | 1.00 18.12 |
| MOTA | 12028 | CA | GLN | 1810 | | -43.943 | 34.978 | 1.00 19.74 |
| MOTA | 12029 | CB | GLN | 1810 | | -43.078 | 35.957 | 1.00 22.02 |
| MOTA | 12030 | CG | GLN | 1810 | | -43.410 | 36.021 | 1.00 24.70 |
| ATOM | 12031 | CD | GLN | 1810 | 25.527 | -43.270 | 34.676 | 1.00 24.85 |
| MOTA | 12032 | | GLN | 1810 | | -44.197 | 33.869 | 1.00 26.62 |
| MOTA | 12033 | NE2 | | 1810 | | -42.101 | 34.430 | 1.00 25.00 |
| MOTA | 12034 | C | GLN | 1810 | | -45.363 | 35.520 | 1.00 20.60 |
| ATOM | 12035 | 0 | GLN | 1810 | | -46.275 | 35.142 | 1.00 19.97 |
| ATOM | 12036 | N | LYS | 1811 | | -45.553 | 36.391 | 1.00 20.73 |
| ATOM | 12037 | CA | LYS | 1811 | | -46.881 | 36.952 | 1.00 22.94 |
| ATOM | 12038 | CB | LYS | 1811 | | -46.825 -48 183 | 37.989 38.647 | 1.00 25.60 1.00 30.12 |
| ATOM | 12039 | CG | LYS | 1811 | 19.688 | -48.183 -48.325 | 39.172 | 1.00 30.12 |
| MOTA | 12040 | CD | LYS | 1811 | 10.433 | -0.040 | JJ. 1/2 | 1.00 04.01 |

| ATOM | 12041 | CE | LYS | 1811 | 17.969 | -47.428 | 40.368 | 1.00 | 37.63 |
|--------------|----------------|----------|------------|--------------|--------|--------------------|------------------|------|----------------|
| ATOM | 12042 | NZ | LYS | 1811 | 16.572 | -47.640 | 40.868 | 1.00 | 38.97 |
| ATOM | 12043 | С | LYS | 1811 | 20.677 | -47.820 | 35.822 | 1.00 | 22.37 |
| ATOM | 12044 | 0 | LYS | 1811 | 21.130 | -48.965 | 35.750 | 1.00 | 23.23 |
| ATOM | 12045 | N | TYR | 1812 | 19.803 | -47.327 | 34.948 | 1.00 | 20.19 |
| MOTA | 12046 | CA | TYR | 1812 | 19.328 | -48.108 | 33.806 | 1.00 | 19.41 |
| MOTA | 12047 | CB | TYR | 1812 | 18.394 | -47.252 | 32.939 | 1.00 | 20.86 |
| ATOM | 12048 | CG | TYR | 1812 | 17.008 | -47.048 | 33.529 | 1.00 | 23.68 |
| ATOM | 12049 | CD1 | TYR | 1812 | 16.100 | -46.165 | 32.941 | 1.00 | 25.01 |
| ATOM | 12050 | CE1 | TYR | 1812 | 14.810 | -46.011 | 33.456 | 1.00 | 28.32 |
| MOTA | 12051 | CD2 | TYR | 1812 | 16.590 | -47.769 | 34.650 | 1.00 | 25.69 |
| MOTA | 12052 | CE2 | TYR | 1812 | 15.307 | -47.623 | 35.169 | 1.00 | 26.94 |
| MOTA | 12053 | CZ | TYR | 1812 | | -46.748 | 34.568 | | 27.83 |
| MOTA | 12054 | ОН | TYR | 1812 | | -46.626 | 35.067 | | 33.55 |
| MOTA | 12055 | С | TYR | 1812 | 20.488 | -48.620 | 32.960 | | 19.49 |
| MOTA | 12056 | 0 | TYR | 1812 | | -49.768 | 32.508 | | 18.51 |
| MOTA | 12057 | N | LYS | 1813 | | -47.768 | 32.739 | | 18.22 |
| MOTA | 12058 | CA | LYS | 1813 | | -48.177 | 31.950 | | 18.58 |
| ATOM | 12059 | CB | LYS | 1813 | 23.577 | -46.993 | 31.679 | | 17.18 |
| MOTA | 12060 | CG | LYS | 1813 | 24.847 | -47.399 | 30.924 | | 14.61 |
| MOTA | 12061 | CD | LYS | 1813 | | -46.214 | 30.288 | | 14.45 |
| MOTA | 12062 | CE | LYS | 1813 | 26.783 | -46.661 | 29.524 | | 13.10 |
| ATOM | 12063 | NZ | LYS | 1813 | 26.884 | -45.976 | 28.193 | | 12.51 |
| MOTA | 12064 | C | LYS | 1813 | | -49.284 | 32.688 | | 19.88 |
| ATOM | 12065 | 0 | LYS | 1813 | | -50.247 | 32.076 | | 19.85 |
| MOTA | 12066 | N | GLN | 1814 | | -49.144 | 34.001 | | 23.03 |
| ATOM | 12067 | CA | GLN | 1814 | | -50.156 | 34.785 | | 26.55 |
| MOTA | 12068 | CB | GLN | 1814 | | -49.695 | 36.229 | | 30.23 |
| MOTA | 12069 | CG | GLN | 1814 | | -48.461 | 36.380 | | 36.91 |
| ATOM | 12070 | CD | GLN | 1814 | | -48.052 | 37.827 | | 40.35 |
| ATOM | 12071 | OE1 | | 1814 | | -48.843 | 38.655 | | 43.65 |
| ATOM | 12072 | NE2 | GLN | 1814 | | -46.811 | 38.142 | | 43.19 26.92 |
| ATOM | 12073 | C | GLN | 1814 | | -51.480 | 34.745 | | |
| MOTA | 12074 | 0 | GLN | 1814 | | -52.553 | 34.697 | | 29.93 26.78 |
| MOTA | 12075 | N | GLU | 1815 | | -51.402 -52.595 | 34.756 34.720 | | 26.76 |
| ATOM | 12076 | CA | GLU GLU | 1815 1815 | | -52.290 | 35.342 | | 29.31 |
| ATOM ATOM | 12077 12078 | CB CG | GLU | 1815 | | -51.678 | 36.735 | | 35.92 |
| ATOM | 12078 | CD | GLU | 1815 | | -51.375 | 37.325 | | 38.20 |
| ATOM | 12079 | OE1 | | 1815 | | -50.624 | 36.694 | | 40.52 |
| ATOM | 12081 | OE2 | | 1815 | 18.352 | -51.886 | 38.424 | | 42.17 |
| ATOM | 12082 | C | GLU | 1815 | 21.118 | -53.075 | 33.285 | | 24.86 |
| ATOM | 12083 | ō | GLU | 1815 | | -54.113 | 33.048 | | 24.50 |
| ATOM | 12084 | N | LYS | 1816 | | -52.318 | 32.331 | | 23.60 |
| MOTA | 12085 | CA | LYS | 1816 | | -52.653 | 30.920 | 1.00 | 24.10 |
| ATOM | 12086 | СВ | LYS | 1816 | | -54.012 | 30.619 | | 27.06 |
| MOTA | 12087 | CG | LYS | 1816 | | -53.956 | 30.494 | 1.00 | 29.88 |
| ATOM | 12088 | CD | LYS | 1816 | | -53.130 | 29.280 | | 33.12 |
| ATOM | 12089 | CE | LYS | 1816 | 25.622 | -52.924 | 29.206 | 1.00 | 34.77 |
| ATOM | 12090 | NZ | LYS | 1816 | 26.378 | -54.205 | 29.060 | 1.00 | 36.10 |
| ATOM | 12091 | С | LYS | 1816 | 20.048 | -52.658 | 30.491 | 1.00 | 23.58 |
| MOTA | 12092 | 0 | LYS | 1816 | 19.635 | -53.456 | 29.650 | 1.00 | 22.90 |
| MOTA | 12093 | N | LYS | 1817 | 19.258 | -51.763 | 31.081 | | 22.10 |
| MOTA | 12094 | CA | LYS | 1817 | 17.847 | -51.649 | 30.730 | 1.00 | 19.64 |
| MOTA | 12095 | CB | LYS | 1817 | 16.982 | -51.432 | 31.973 | | 23.35 |
| MOTA | 12096 | CG | LYS | 1817 | 15.498 | -51.274 | 31.636 | 1.00 | 26.44 |
| MOTA | 12097 | CD | LYS | 1817 | | -50.726 | 32.801 | | 30.23 |
| MOTA | 12098 | CE | LYS | 1817 | | -51.683 | 33.980 | | 33.21 |
| MOTA | 12099 | NZ | LYS | 1817 | | -51.115 | 35.101 | | 36.99 |
| MOTA | 12100 | С | LYS | 1817 | | -50.463 | 29.790 | | 19.22 |
| MOTA | 12101 | 0 | LYS | 1817 | | -49.311 | 30.212 | | 15.14 |
| MOTA | 12102 | N | ARG | 1818 | | -50.756 | 28.523 | | 17.56 |
| MOTA | 12103 | CA | ARG | 1818 | | -49.723 | 27.515 | | 17.68 |
| ATOM | 12104 | CB | ARG | 1818 | | -50.354 | 26.121 | | 17.01 |
| ATOM | 12105 | CG | ARG | 1818 | | -50.558 | 25.563 | | 20.64 |
| ATOM | 12106 | CD | ARG | 1818 | | -51.433 | 24.331 | | 26.16 |
| ATOM | 12107 | NE | ARG | 1818 | | -52.836 | 24.671 | | 27.97 |
| ATOM | 12108 | CZ | ARG | 1818 | | -53.847 | 23.833 | | 30.30 |
| MOTA | 12109 | | ARG | 1818 | | -53.611 | 22.602 | | 31.08 |
| MOTA | 12110 | | ARG | 1818 | | -55.091 | 24.223 | | 30.79 |
| MOTA | 12111 | С | ARG | 1818 | | -48.939 -49.522 | 27.800 28.107 | | 16.78 |
| ATOM | 12112 | O N | ARG | 1818 | | -49.522 -47.615 | 28.107 | | 17.29 15.71 |
| MOTA | 12113 | N | PHE | 1819 | | -47.615 -46.764 | 28.005 | | 13.45 |
| MOTA MOTA | 12114 12115 | CA CB | PHE PHE | 1819 1819 | | -46.764 -45.940 | 28.005 | | 12.38 |
| ATOM | 12116 | CG | PHE | 1819 | | -45.082 | 29.135 | | 10.54 |
| ATOM | 12117 | | PHE | 1819 | | -43.780 | 28.653 | | 10.46 |
| | 1011/ | CDI | 1112 | 1019 | 10.502 | 45.700 | 20.000 | | |

| ATOM | 12118 | CD2 | PHE | 1819 | 17.648 | -45.576 | 29.494 | 1.00 | 11.28 |
|------|-------|-----|-------|------|--------|---------|------------------|------|-------|
| ATOM | | CE1 | PHE | 1819 | 17.434 | -42.980 | 28.540 | 1.00 | 10.02 |
| ATOM | | | PHE | 1819 | | -44.782 | 29.384 | | 12.19 |
| ATOM | | CZ | PHE | 1819 | | -43.484 | 28.903 | 1.00 | 10.00 |
| ATOM | | C | PHE | 1819 | 14.405 | -45.848 | 26.877 | 1.00 | 12.26 |
| ATOM | | Ö | PHE | 1819 | | -45.404 | 26.057 | | 11.06 |
| ATOM | | N | ALA | 1820 | | -45.572 | 26.850 | | 11.30 |
| | | | ALA | 1820 | | -44.715 | 25.833 | | 11.83 |
| ATOM | | CA | | | | | | | 10.93 |
| ATOM | | CB | ALA | 1820 | | -45.203 | 25.470 | | |
| ATOM | | С | ALA | 1820 | | -43.256 | 26.262 | | 11.52 |
| ATOM | | 0 | ALA | 1820 | | -42.945 | 27.441 | | 13.43 |
| ATOM | | N | THR | 1821 | | -42.372 | 25.277 | | 11.00 |
| ATOM | | CA | THR | 1821 | | -40.928 | 25.481 | | 11.82 |
| ATOM | | CB | THR | 1821 | | -40.321 | 25.403 | | 11.47 |
| ATOM | 12132 | OG1 | THR | 1821 | 14.756 | -40.809 | 26.505 | | 15.36 |
| ATOM | 12133 | CG2 | THR | 1821 | 13.913 | -38.816 | 25.451 | 1.00 | 23.24 |
| ATOM | 12134 | С | THR | 1821 | 11.706 | -40.398 | 24.331 | 1.00 | 9.33 |
| ATOM | 12135 | 0 | THR | 1821 | 11.554 | -41:075 | 23.312 | 1.00 | 12.52 |
| ATOM | 12136 | N | ILE | 1822 | 11.150 | -39.201 | 24.465 | 1.00 | 10.58 |
| ATOM | 12137 | CA | ILE | 1822 | 10.315 | -38.690 | 23.385 | 1.00 | 9.32 |
| ATOM | | CB | ILE | 1822 | 8.892 | -39.296 | 23.504 | 1.00 | 10.75 |
| ATOM | | CG2 | ILE | 1822 | 8.162 | -38.672 | 24.716 | 1.00 | 10.54 |
| ATOM | | | ILE | 1822 | | -39.050 | 22.222 | 1.00 | 13.24 |
| ATOM | | | ILE | 1822 | | -39.836 | 22.165 | | 14.23 |
| ATOM | | C | ILE | 1822 | | -37.169 | 23.415 | | 12.04 |
| ATOM | | Õ | ILE | 1822 | | -36.552 | 24.456 | 1.00 | 9.11 |
| ATOM | | N | THR | 1823 | | -36.565 | 22.269 | | 10.88 |
| | | | THR | | | -35.119 | 22.212 | 1.00 | 12.73 |
| ATOM | | CA | | 1823 | | -34.570 | 20.766 | 1.00 | 11.54 |
| ATOM | | CB | THR | 1823 | | | | | |
| ATOM | | | THR | 1823 | | -35.126 | 19.889 | | 12.04 |
| ATOM | | | THR | 1823 | | -34.936 | 20.259 | | 14.24 |
| ATOM | | C | THR | 1823 | | -34.785 | 22.681 | 1.00 | |
| ATOM | | 0 | THR | 1823 | | -35.591 | 22.546 | 1.00 | 11.41 |
| ATOM | | N | ALA | 1824 | | -33.599 | 23.257 | | 10.84 |
| ATOM | | CA | ALA | 1824 | | -33.134 | 23.756 | 1.00 | 10.40 |
| ATOM | 12153 | CB | ALA | 1824 | | -33.673 | 25.173 | 1.00 | 9.05 |
| ATOM | 12154 | C | ALA | 1824 | 6.973 | -31.604 | 23.776 | | 10.44 |
| ATOM | 12155 | 0 | ALA | 1824 | 8.015 | -31.023 | 24.087 | 1.00 | 9.73 |
| ATOM | 12156 | N | TYR | 1825 | 5.867 | -30.947 | 23.445 | 1.00 | 9.09 |
| ATOM | 12157 | CA | TYR | 1825 | 5.864 | -29.483 | 23.405 | 1.00 | 10.72 |
| ATOM | 12158 | CB | TYR | 1825 | 6.002 | -28.995 | 21.960 | 1.00 | 9.65 |
| ATOM | | CG | TYR | 1825 | 7.028 | -29.745 | 21.159 | 1.00 | 10.96 |
| ATOM | | | TYR | 1825 | | -30.696 | 20.226 | | 13.24 |
| ATOM | | | TYR | 1825 | | -31.379 | 19.466 | 1.00 | |
| АТОМ | | | TYR | 1825 | | -29.496 | 21.323 | | 11.25 |
| ATOM | | | TYR | 1825 | | -30.180 | 20.569 | | 10.63 |
| ATOM | | CZ | TYR | 1825 | | -31.116 | 19.642 | | 12.50 |
| ATOM | | OH | TYR | 1825 | | -31.782 | 18.876 | | 13.92 |
| ATOM | | C | TYR | 1825 | | -28.854 | 23.994 | 1.00 | 11.54 |
| | | | TYR | | 4.427 | -27.642 | | 1.00 | 12.75 |
| ATOM | | 0 | | 1825 | | -27.642 | 23.906 24.592 | 1.00 | 9.86 |
| ATOM | | N | ASP | 1826 | | | | | |
| ATOM | | CA | | 1826 | | -29.141 | 25.170 | | 12.59 |
| ATOM | | CB | ASP | 1826 | | -29.020 | 24.084 | | 10.93 |
| ATOM | | CG | ASP | 1826 | | -30.362 | 23.471 | | 13.46 |
| ATOM | | OD1 | | 1826 | | -31.125 | 24.116 | | 12.97 |
| ATOM | | OD2 | | 1826 | | -30.656 | 22.356 | | 14.57 |
| ATOM | | C | ASP | 1826 | | -30.007 | 26.325 | | 11.01 |
| ATOM | | 0 | ASP | 1826 | | -31.120 | 26.549 | | 12.69 |
| ATOM | | N | TYR | 1827 | | -29.469 | 27.060 | | 11.39 |
| ATOM | | CA | TYR | 1827 | | -30.145 | 28.212 | | 11.45 |
| MOTA | 12178 | CB | TYR | 1827 | -0.513 | -29.212 | 28.879 | | 12.27 |
| ATOM | 12179 | CG | TYR | 1827 | -1.358 | -29.886 | 29.937 | | 12.69 |
| ATOM | 12180 | CD1 | TYR | 1827 | -0.912 | -29.990 | 31.255 | | 14.43 |
| ATOM | | CE1 | TYR | 1827 | | -30.593 | 32.234 | | 15.64 |
| ATOM | | CD2 | TYR | 1827 | | -30.407 | 29.622 | 1.00 | 14.53 |
| ATOM | | | TYR | 1827 | -3.401 | -31.015 | 30.593 | 1.00 | 17.16 |
| ATOM | | CZ | TYR | 1827 | | -31.101 | 31.893 | 1.00 | 16.99 |
| ATOM | | OH | TYR | 1827 | | -31.686 | 32.861 | 1.00 | 16.74 |
| ATOM | | C | TYR | 1827 | | -31.483 | 27.921 | | 11.79 |
| АТОМ | | ō | TYR | 1827 | | -32.474 | 28.632 | | 10.69 |
| ATOM | | N | SER | 1828 | | -31.506 | 26.887 | 1.00 | 9.98 |
| ATOM | | CA | SER | 1828 | | -32.713 | 26.553 | | 12.49 |
| ATOM | | CB | SER | 1828 | | -32.415 | 25.407 | | 11.71 |
| ATOM | | OG | SER | 1828 | | -31.420 | 25.819 | | 16.55 |
| ATOM | | C | SER | 1828 | | -33.940 | 26.240 | | 11.86 |
| ATOM | | 0 | SER | 1828 | | -35.027 | 26.763 | | 9.82 |
| ATOM | | N | PHE | 1829 | | -33.780 | 25.401 | | 11.47 |
| AIOM | 12194 | IN | £ 11E | 1029 | 0.075 | 55.700 | 20.401 | 1.00 | |
| | | | | | | | | | |

| ATOM | 12195 | CA | PHE | 1829 | 0.921 -34.918 | 25.082 | 1.00 11.15 |
|--------------|----------------|----------|------------|--------------|----------------------------------|------------------|--------------------------|
| ATOM | 12196 | CB | PHE | 1829 | 1.675 -34.690 | 23.760 | 1.00 10.81 |
| ATOM | 12197 | CG | PHE | 1829 | 0.831 -34.948 | 22.535 | 1.00 10.15 |
| MOTA | 12198 | CD1 | PHE | 1829 | 0.259 -33.893 | 21.827 | 1.00 10.05 |
| MOTA | 12199 | CD2 | PHE | 1829 | 0.566 -36.256 | 22.120 | 1.00 9.31 |
| MOTA | 12200 | CE1 | PHE | 1829 | -0.570 -34.134 | 20.723 | 1.00 9.40 |
| MOTA | 12201 | CE2 | PHE | 1829 | -0.259 -36.512 | 21.022 | 1.00 10.09 |
| MOTA | 12202 | CZ | PHE | 1829 | -0.831 -35.451 | 20.317 | 1.00 9.43 |
| MOTA | 12203 | С | PHE | 1829 | 1.882 -35.224 | 26.241 | 1.00 11.61 |
| MOTA | 12204 | 0 | PHE | 1829 | 2.161 -36.391 | 26.531 | 1.00 9.86 |
| ATOM | 12205 | N | ALA | 1830 | 2.366 -34.199 | 26.939 | 1.00 9.53 |
| MOTA | 12206 | CA | ALA | 1830 | 3.269 -34.475 | 28.057 | 1.00 11.06 |
| ATOM | 12207 | СВ | ALA | 1830 | 3.810 -33.168 | 28.663 | 1.00 13.38 |
| ATOM | 12208 | С | ALA | 1830 | 2.535 -35.284 | 29.131 | 1.00 12.72 |
| ATOM | 12209 | 0 | ALA | 1830 | 3.116 -36.172 | 29.759 | 1.00 12.34 |
| ATOM | 12210 | N | LYS | 1831 | 1.260 -34.963 | 29.336 | 1.00 10.44 |
| MOTA | 12211 | CA | LYS | 1831 | 0.435 -35.645 | 30.324 | 1.00 12.92 1.00 15.79 |
| ATOM | 12212 | CB | LYS | 1831 1831 | -0.884 -34.886 -1.892 -35.560 | 30.502 31.418 | 1.00 15.79 |
| ATOM ATOM | 12213 12214 | CG CD | LYS LYS | 1831 | -1.386 -35.636 | 32.837 | 1.00 19.79 |
| ATOM | 12214 | CE | LYS | 1831 | -2.551 -35.751 | 33.817 | 1.00 20.44 |
| ATOM | 12215 | NZ | LYS | 1831 | -3.543 -36.796 | 33.410 | 1.00 30.54 |
| MOTA | 12217 | C | LYS | 1831 | 0.151 -37.071 | 29.866 | 1.00 10.03 |
| ATOM | 12218 | ō | LYS | 1831 | 0.202 -38.026 | 30.658 | 1.00 10.29 |
| ATOM | 12219 | N | LEU | 1832 | -0.158 -37.211 | 28.582 | 1.00 9.47 |
| ATOM | 12220 | CA | LEU | 1832 | -0.449 -38.529 | 28.017 | 1.00 10.13 |
| ATOM | 12221 | CB | LEU | 1832 | -0.811 -38.397 | 26.532 | 1.00 9.08 |
| ATOM | 12222 | CG | LEU | 1832 | -1.337 -39.651 | 25.819 | 1.00 7.77 |
| ATOM | 12223 | CD1 | LEU | 1832 | -2.165 -39.212 | 24.629 | 1.00 10.73 |
| ATOM | 12224 | CD2 | LEU | 1832 | -0.187 -40.548 | 25.370 | 1.00 8.84 |
| ATOM | 12225 | С | LEU | 1832 | 0.764 -39.434 | 28.195 | 1.00 11.17 |
| ATOM | 12226 | 0 | LEU | 1832 | 0.632 -40.583 | 28.619 | 1.00 10.67 |
| ATOM | 12227 | N | PHE | 1833 | 1.948 -38.907 | 27.888 | 1.00 9.31 |
| ATOM | 12228 | CA | PHE | 1833 | 3.175 -39.690 | 28.021 | 1.00 10.32 |
| MOTA | 12229 | CB | PHE | 1833 | 4.385 -38.928 | 27.453 | 1.00 12.77 |
| ATOM | 12230 | CG | PHE | 1833 | 4.253 -38.554 | 25.983 | 1.00 10.12 |
| ATOM | 12231 | | PHE | 1833 | 3.502 -39.331 | 25.105 | 1.00 9.09 |
| ATOM | 12232 | | PHE | 1833 | 4.898 -37.427 | 25.483 | 1.00 11.46 |
| ATOM | 12233 | CE1 | PHE | 1833 | 3.393 -38.989 | 23.746 | 1.00 9.84 |
| ATOM | 12234 | CE2 | PHE | 1833 | 4.798 -37.074 | 24.125 | 1.00 9.94 |
| MOTA | 12235 | CZ | PHE | 1833 | 4.041 -37.860 | 23.254 | 1.00 8.51 |
| ATOM | 12236 | C | PHE | 1833 | 3.438 -40.043 | 29.486 | 1.00 11.08 |
| ATOM | 12237 | 0 | PHE | 1833 | 3.687 -41.204 3.392 -39.045 | 29.810 30.369 | 1.00 11.34 1.00 11.64 |
| MOTA | 12238 12239 | N CA | ALA ALA | 1834 1834 | 3.631 -39.285 | 31.792 | 1.00 11.04 |
| ATOM ATOM | 12240 | CB | ALA | 1834 | 3.480 -37.973 | 32.590 | 1.00 12.34 |
| ATOM | 12241 | С | ALA | 1834 | 2.692 -40.349 | 32.367 | 1.00 13.95 |
| ATOM | 12242 | 0 | ALA | 1834 | 3.120 -41.206 | 33.150 | 1.00 13.96 |
| ATOM | 12243 | N | ASP | 1835 | 1.419 -40.313 | 31.981 | 1.00 14.27 |
| ATOM | 12244 | CA | ASP | 1835 | 0.468 -41.290 | 32.501 | 1.00 16.50 |
| ATOM | 12245 | CB | ASP | 1835 | -0.968 -40.917 | 32.133 | 1.00 20.28 |
| ATOM | 12246 | CG | ASP | 1835 | -1.457 -39.671 | | • |
| MOTA | 12247 | | ASP | 1835 | -0.859 -39.275 | 33.875 | 1.00 22.29 |
| MOTA | 12248 | | ASP | 1835 | -2.457 -39.096 | 32.388 | 1.00 25.23 |
| MOTA | 12249 | C | ASP | 1835 | 0.734 -42.723 | 32.048 | 1.00 16.31 |
| MOTA | 12250 | 0 | ASP | 1835 | 0.176 -43.671 | 32.612 | 1.00 14.66 |
| ATOM | 12251 | N | GLU | 1836 | 1.571 -42.891 | 31.028 | 1.00 15.72 |
| MOTA | 12252 | CA | GLU | 1836 | 1.905 -44.234 | 30.557 | 1.00 14.86 |
| MOTA | 12253 | CB | GLU . | | 1.966 -44.289 | 29.024 | 1.00 13.08 |
| ATOM | 12254 | CG | GLU | 1836 | 0.634 -44.045 | 28.334 | 1.00 13.80 |
| ATOM | 12255 | CD | GLU | 1836 | -0.468 -44.917 | 28.905 | 1.00 18.45 |
| MOTA | 12256 | | GLU | 1836 | -0.22146.126 | 29.116 | 1.00 18.78 |
| ATOM | 12257 | | GLU | 1836 | -1.578 -44.395 | 29.144 | 1.00 18.26 |
| ATOM | 12258 | C | GLU | 1836 | 3.246 -44.688 | 31.123 | 1.00 15.46 |
| ATOM | 12259 | 0 | GLU | 1836 1837 | 3.632 -45.844 | 30.970 | 1.00 16.15 1.00 13.82 |
| ATOM ATOM | 12260 12261 | N CA | GLY | 1837 | 3.962 -43.770 5.252 -44.112 | 31.762 32.336 | 1.00 13.82 |
| ATOM | 12262 | CA | GLY GLY | 1837 | 6.442 -43.693 | 31.494 | 1.00 14.40 |
| ATOM | 12262 | 0 | GLY | 1837 | 7.567 -44.113 | 31.761 | 1.00 14.75 |
| ATOM | 12264 | N | LEU | 1838 | 6.197 -42.879 | 30.466 | 1.00 14.75 |
| ATOM | 12265 | CA | LEU | 1838 | 7.263 -42.384 | 29.588 | 1.00 14.07 |
| ATOM | 12266 | CB | LEU | 1838 | 6.703 -42.123 | 28.188 | 1.00 18.28 |
| ATOM | 12267 | CG | LEU | 1838 | 7.637 -42.371 | 27.005 | 1.00 21.26 |
| ATOM | 12268 | | LEU | 1838 | 6.977 -41.842 | 25.744 | 1.00 18.89 |
| ATOM | 12269 | | LEU | 1838 | 8.983 -41.721 | 27.225 | 1.00 20.44 |
| MOTA | 12270 | С | LEU | 1838 | 7.642 -41.073 | 30.267 | 1.00 17.17 |
| MOTA | 12271 | 0 | LEU | 1838 | 7.054 -40.024 | 29.987 | 1.00 16.93 |
| | | | | | | | |

| ATOM | 12272 | N | ASN | 1839 | 8.632 - | 41.160 | 31.152 | 1.00 | 19.21 |
|--------------|----------------|----------|------------|--------------|---------------------|------------------|------------------|------|--------------|
| ATOM | 12273 | CA | ASN | 1839 | 9.066 - | 40.046 | 31.981 | 1.00 | 17.01 |
| ATOM | 12274 | CB | ASN | 1839 | 9.234 - | 40.551 | 33.423 | 1.00 | 20.88 |
| ATOM | 12275 | CG | ASN | 1839 | 8.011 - | 41.318 | 33.927 | 1.00 | 24.27 |
| ATOM | 12276 | | ASN | 1839 | 6.867 - | 40.885 | 33.742 | 1.00 | 27.75 |
| ATOM | 12277 | ND2 | ASN | 1839 | 8.248 - | 42.452 | 34.577 | 1.00 | 26.34 |
| ATOM | 12278 | С | ASN | 1839 | 10.317 - | 39.276 | 31.567 | 1.00 | 15.58 |
| MOTA | 12279 | 0 | ASN | 1839 | 10.956 - | 38.627 | 32.397 | 1.00 | 15.41 |
| MOTA | 12280 | N | VAL | 1840 | 10.684 - | 39.347 | 30.296 | 1.00 | 14.55 |
| ATOM | 12281 | CA | VAL | 1840 | 11.841 - | 38.607 | 29.830 | 1.00 | 13.23 |
| MOTA | 12282 | CB | VAL | 1840 | 13.027 - | 39.528 | 29.518 | 1.00 | 13.11 |
| ATOM | 12283 | CG1 | VAL | 1840 | 14.221 - | 38.694 | 29.118 | 1.00 | 13.44 |
| MOTA | 12284 | CG2 | VAL | 1840 | 13.348 - | 40.392 | 30.748 | 1.00 | 16.08 |
| MOTA | 12285 | С | VAL | 1840 | 11.409 - | 37.884 | 28.573 | 1.00 | 12.06 |
| MOTA | 12286 | 0 | VAL | 1840 | 11.116 - | 38.505 | 27.547 | 1.00 | 10.12 |
| ATOM | 12287 | N | MET | 1841 | 11.367 - | 36.562 | 28.663 | 1.00 | 10.19 |
| ATOM | 12288 | CA | MET | 1841 | 10.909 - | 35.758 | 27.548 | 1.00 | 10.11 |
| MOTA | 12289 | CB | MET | 1841 | 9.522 - | 35.193 | 27.873 | 1.00 | 12.54 |
| ATOM | 12290 | CG | MET | 1841 | 8.452 - | 36.273 | 27.916 | 1.00 | 15.69 |
| ATOM | 12291 | SD | MET | 1841 | 6.923 - | 35.649 | 28.511 | 1.00 | 15.98 |
| MOTA | 12292 | CE | MET | 1841 | 6.633 - | 36.759 | 29.903 | 1.00 | 13.37 |
| MOTA | 12293 | С | MET | 1841 | 11.864 - | 34.647 | 27.150 | 1.00 | 10.13 |
| MOTA | 12294 | 0 | MET | 1841 | 12.468 ~ | 33.969 | 27.992 | 1.00 | 9.95 |
| MOTA | 12295 | N | LEU | 1842 | 11.959 - | 34.456 | 25.839 | 1.00 | 10.43 |
| MOTA | 12296 | CA | LEU | 1842 | 12.838 - | 33.454 | 25.264 | 1.00 | 11.43 |
| MOTA | 12297 | CB | LEU | 1842 | 13.804 - | 34.123 | 24.283 | 1.00 | |
| MOTA | 12298 | CG | LEU | 1842 | 14.979 - | 33.359 | 23.651 | 1.00 | 20.32 |
| MOTA | 12299 | CD1 | LEU | 1842 | 14.650 - | 33.033 | 22.220 | | 23.15 |
| MOTA | 12300 | CD2 | LEU | 1842 | 15.339 - | 32.102 | 24.428 | 1.00 | 19.90 |
| MOTA | 12301 | C | LEU | 1842 | 12.060 - | 32.349 | 24.566 | 1.00 | 11.63 |
| MOTA | 12302 | 0 | LEU | 1842 | 11.246 - | 32.610 | 23.687 | 1.00 | 9.65 |
| MOTA | 12303 | N | VAL | 1843 | 12.299 - | 31.115 | 25.001 | 1.00 | 11.18 |
| MOTA | 12304 | CA | VAL | 1843 | 11.670 - | 29.947 | 24.395 | 1.00 | 12.10 |
| MOTA | 12305 | CB | VAL | 1843 | 11.215 - | 28.917 | 25.454 | 1.00 | 12.21 |
| MOTA | 12306 | CG1 | VAL | 1843 | 10.567 - | 27.708 | 24.763 | 1.00 | |
| MOTA | 12307 | CG2 | VAL | 1843 | 10.212 - | 29.564 | 26.405 | 1.00 | |
| MOTA | 12308 | C | VAL | 1843 | 12.800 - | 29.383 | 23.548 | 1.00 | |
| MOTA | 12309 | О | VAL | 1843 | 13.601 - | 28.580 | 24.019 | 1.00 | |
| MOTA | 12310 | N | GLY | 1844 | | 29.837 | 22.302 | 1.00 | |
| MOTA | 12311 | CA | GLY | 1844 | | 29.406 | 21.424 | 1.00 | |
| MOTA | 12312 | С | GLY | 1844 | | 28.393 | 20.375 | 1.00 | |
| ATOM | 12313 | .0 | GLY | 1844 | | 28.167 | 20.127 | 1.00 | |
| MOTA | 12314 | N | ASP | 1845 | 14.559 - | | 19.742 | 1.00 | |
| ATOM | 12315 | CA | ASP | 1845 | 14.246 - | | 18.732 | 1.00 | |
| MOTA | 12316 | CB | ASP | 1845 | | 25.952 | 18.342 | 1.00 | |
| MOTA | 12317 | CG | ASP | 1845 | | 26.794 | 17.857 | 1.00 | |
| MOTA | 12318 | | ASP | 1845 | | 27.985 | 17.559 | 1.00 | |
| MOTA | 12319 | OD2 | ASP | 1845 | | 26.227 | 17.768 | 1.00 | |
| MOTA | 12320 | С | ASP | 1845 | | 27.368 | 17.506 | 1.00 | |
| ATOM | 12321 | 0 | ASP | 1845 | | 26.641 | 16.588 | 1.00 | 14.70 |
| MOTA | 12322 | N | SER | 1846 | | 28.689 | 17.493 | 1.00 | |
| MOTA | 12323 | CA | SER | 1846 | 12.699 - | | 16.385 | | 12.45 |
| MOTA | 12324 | CB | SER | 1846 | 12.615 - | | 16.607 | | 14.08 |
| MOTA | 12325 | OG | SER | 1846 | 12.079 - | | 17.888 | 1.00 | |
| MOTA | 12326 | C | SER | 1846 | | 28.735 | 16.337 | 1.00 | 12.85 |
| ATOM | 12327 | 0 | SER | 1846 | | 28.821 | 15.316 | | 13.17 |
| ATOM | 12328 | N | LEU | 1847 | | 28.146 | 17.451 | | 9.80 |
| ATOM | 12329 | CA | LEU | 1847 | | 27.517 | 17.503 | 1.00 | |
| ATOM | 12330 | CB | LEU | 1847 | | 26.969 | 18.911 | 1.00 | 8.90 |
| ATOM | 12331 | CG | LEU | 1847 | | 25.770 | 19.432 | 1.00 | 9.46 |
| MOTA | 12332 | | LEU | 1847 | | 24.474 | 18.904 | | 6.94 |
| ATOM | 12333 | | LEU | 1847 | 10.039 - | | 20.968 | | |
| ATOM | 12334 | C | LEU | 1847 | 9.436 - | | 16.466 | 1.00 | 8.37 9.72 |
| ATOM | 12335 | O N | LEU | 1847 | | 26.001 25.861 | 16.051 16.060 | 1.00 | 7.80 |
| MOTA | 12336 | N | GLY | 1848 | | | 15.061 | 1.00 | 9.90 |
| MOTA | 12337 | CA | GLY | 1848 | 10.594 - 9.921 - | 25.270 | 13.783 | | 12.28 |
| MOTA | 12338 | C | GLY | 1848 | 9.921 - 9.277 - | | 13.763 | 1.00 | |
| MOTA | 12339 | O N | GLY | 1848 | 10.048 - | | 13.485 | 1.00 | |
| MOTA | 12340 | N | MET | 1849 | 9.446 - | | 12.273 | | 14.41 |
| MOTA | 12341 | CA | MET | 1849 | 10.406 - | | 11.641 | 1.00 | |
| ATOM ATOM | 12342 12343 | CB CG | MET MET | 1849 1849 | 11.766 - | | 11.327 | | 19.85 |
| ATOM | 12343 | SD | MET . | 1849 | 12.956 - | | 10.655 | | 24.17 |
| MOTA | | CE | MET | 1849 | 12.389 - | | 8.968 | | 24.76 |
| ATOM | 12345 12346 | CE | MET | 1849 | | 27.724 | 12.538 | | 12.05 |
| ATOM | 12346 | 0 | MET | 1849 | 7.097 - | | 11.893 | | 13.07 |
| ATOM | 12347 | N | THR | 1850 | 8.052 - | | 13.518 | | 13.89 |
| 011 | 72340 | -4 | - 111/ | -050 | J. 052 | | | | |

| ATOM | 12349 | CA | THR | 1850 | 6.826 | -29.321 | 13.852 | 1.00 13.07 |
|--------------|----------------|------------|------------|--------------|--------|--------------------|------------------|--------------------------|
| ATOM | 12350 | CB | THR | 1850 | 7.165 | -30.523 | 14.756 | 1.00 16.49 |
| ATOM | 12351 | OG1 | THR | 1850 | 6.003 | -31.332 | 14.935 | 1.00 23.16 |
| MOTA | 12352 | CG2 | THR | 1850 | 7.657 | -30.044 | 16.106 | 1.00 13.78 |
| ATOM | 12353 | C | THR | 1850 | 5.722 | -28.477 | 14.502 | 1.00 13.45 |
| ATOM | 12354 | 0 | THR | 1850 | | -28.704 | 14.272 | 1.00 14.06 |
| ATOM | 12355 | N | VAL | 1851 | 6.101 | -27.505 | 15.318 | 1.00 9.38 |
| MOTA | 12356 | CA | VAL | 1851 | 5.095 | -26.662 | 15.963 | 1.00 10.18 |
| ATOM | 12357 | CB | VAL | 1851 | 5.447 | -26.405 | 17.456 | 1.00 9.38 |
| MOTA | 12358 | CG1 | VAL | 1851 | 4.436 | -25.440 | 18.073 | 1.00 9.31 |
| ATOM | 12359 | CG2 | VAL | 1851 | | -27.719 | 18.219 | 1.00 9.77 |
| MOTA | 12360 | С | VAL | 1851 | | -25.316 | 15.262 | 1.00 10.37 |
| MOTA | 12361 | 0 | VAL | 1851 | | -24.940 | 14.935 | 1.00 10.77 |
| ATOM | 12362 | N | GLN | 1852 | | -24.604 | 15.025 | 1.00 9.98 |
| ATOM | 12363 | CA | GLN | 1852 | | -23.283 | 14.405 | 1.00 10.14 |
| ATOM | 12364 | CB | GLN | 1852 | | -22.486 | 14.801 | 1.00 10.92 |
| ATOM | 12365 | CG | GLN | 1852 | | -22.402 | 16.313 | 1.00 11.64 |
| ATOM | 12366 | CD | GLN | 1852 | | -21.591 | 16.702 | 1.00 11.56 1.00 11.26 |
| ATOM | 12367 | OE1 NE2 | | 1852 | | -21.530 -20.990 | 15.963 17.882 | 1.00 11.26 1.00 8.34 |
| ATOM | 12368 12369 | NE2 | GLN GLN | 1852 1852 | | -20.990 | 12.891 | 1.00 8.34 |
| ATOM ATOM | 12370 | 0 | GLN | 1852 | | -23.277 | 12.315 | 1.00 10.45 |
| ATOM | 12370 | N | GLY | 1853 | | -22.314 -24.340 | 12.239 | 1.00 10.43 |
| ATOM | 12371 | CA | GLY | 1853 | | -24.422 | 10.793 | 1.00 10.59 |
| ATOM | 12372 | C | GLY | 1853 | | -23.823 | 9.941 | 1.00 11.71 |
| ATOM | 12374 | o | GLY | 1853 | | -23.534 | 8.766 | 1.00 12.91 |
| ATOM | 12375 | N | HIS | 1854 | | -23.618 | 10.522 | 1.00 11.61 |
| ATOM | 12376 | CA | HIS | 1854 | | -23.076 | 9.768 | 1.00 14.51 |
| MOTA | 12377 | СВ | HIS | 1854 | | -22.413 | 10.704 | 1.00 12.24 |
| ATOM | 12378 | CG | HIS | 1854 | | -21.230 | 11.432 | 1.00 13.00 |
| ATOM | 12379 | | HIS | 1854 | | -21.033 | 12.747 | 1.00 11.78 |
| ATOM | 12380 | ND1 | HIS | 1854 | 9.636 | -20.060 | 10.792 | 1.00 11.06 |
| ATOM | 12381 | CE1 | HIS | 1854 | 9.186 | -19.193 | 11.682 | 1.00 13.39 |
| MOTA | 12382 | NE2 | HIS | 1854 | 9.231 | -19.758 | 12.875 | 1.00 12.54 |
| ATOM | 12383 | C | HIS | 1854 | 10.210 | -24.225 | 9.037 | 1.00 15.33 |
| MOTA | 12384 | 0 | HIS | 1854 | 10.034 | -25.389 | 9.395 | 1.00 14.84 |
| MOTA | 12385 | N | ASP | 1855 | | -23.888 | 8.028 | 1.00 18.03 |
| MOTA | 12386 | CA | ASP | 1855 | | -24.871 | 7.224 | 1.00 20.65 |
| MOTA | 12387 | CB | ASP | 1855 | | -24.247 | 5.871 | 1.00 26.04 |
| ATOM | 12388 | CG | ASP | 1855 | | -23.172 | 5.999 | 1.00 27.76 |
| ATOM | 12389 | | ASP | 1855 | | -23.526 | 6.253 | 1.00 35.96 |
| ATOM | 12390 | OD2 | | 1855 | | -21.977 | 5.864 | 1.00 34.52 |
| ATOM | 12391 | C | ASP | 1855 | 12.993 | | 7.928 | 1.00 19.44 |
| ATOM | 12392 | 0 | ASP | 1855 | | -26.288 -24.685 | 7.477 9.026 | 1.00 17.58 1.00 17.83 |
| MOTA | 12393 12394 | N CA | SER SER | 1856 1856 | | -25.050 | 9.794 | 1.00 17.03 |
| MOTA MOTA | 12394 | CB | SER | 1856 | | -24.257 | 9.323 | 1.00 15.27 |
| MOTA | 12396 | OG | SER | 1856 | | -22.953 | 9.884 | 1.00 13.49 |
| ATOM | 12397 | C | SER | 1856 | | -24.735 | 11.260 | 1.00 14.46 |
| ATOM | 12398 | Ö | SER | 1856 | | -24.163 | 11.613 | 1.00 13.21 |
| ATOM | 12399 | N | THR | 1857 | | -25.085 | 12.111 | 1.00 15.25 |
| ATOM | 12400 | CA | THR | 1857 | | -24.823 | 13.536 | 1.00 14.62 |
| ATOM | 12401 | CB | THR | 1857 | | -25.947 | 14.392 | 1.00 15.79 |
| ATOM | 12402 | OG1 | | 1857 | | -25.993 | 14.169 | 1.00 14.91 |
| ATOM | 12403 | CG2 | THR | 1857 | 15.106 | -27.286 | 14.042 | 1.00 15.97 |
| MOTA | 12404 | С | THR | 1857 | | -23.516 | 13.964 | 1.00 12.81 |
| ATOM | 12405 | 0 | THR | 1857 | | -23.145 | 15.128 | 1.00 13.80 |
| ATOM | 12406 | N | LEU | 1858 | | -22.815 | 13.047 | 1.00 12.35 |
| MOTA | 12407 | CA | LEU | 1858 | | -21.582 | 13.434 | 1.00 12.54 |
| ATOM | 12408 | CB | LEU | 1858 | | -21.013 | 12.252 | 1.00 12.41 |
| MOTA | 12409 | CG | LEU | 1858 | | -21.743 | 11.959 | 1.00 18.92 |
| MOTA | 12410 | | LEU | 1858 | | -23.123 | 11.376 | 1.00 18.27 |
| ATOM | 12411 | | LEU | 1858 | | -20.929 | 10.975 | 1.00 16.42 |
| ATOM | 12412 | C | LEU | 1858 | | -20.465 -19.749 | 14.049 14.943 | 1.00 12.00 1.00 12.79 |
| MOTA | 12413 | 0 | LEU | 1858 | | | 13.587 | 1.00 12.79 |
| ATOM | 12414 | N CD | PRO PRO | 1859 1859 | | -20.296 -20.851 | 12.366 | 1.00 11.97 |
| MOTA MOTA | 12415 12416 | CA | | . 1859 | | -19.228 | 14.159 | 1.00 13.30 |
| ATOM | 12417 | CB. | PRO | 1859 | | -19.178 | 13.222 | 1.00 12.67 |
| ATOM | 12417 | CG | PRO | 1859 | | -20.528 | 12.567 | 1.00 20.26 |
| ATOM | 12418 | C | PRO | 1859 | | -19.393 | 15.623 | 1.00 20.20 |
| ATOM | 12420 | 0 | PRO | 1859 | | -18.418 | 16.287 | 1.00 11.90 |
| ATOM | 12421 | Ņ | VAL | 1860 | | -20.620 | 16.125 | 1.00 9.89 |
| ATOM | 12422 | CA | VAL | 1860 | | -20.900 | 17.514 | 1.00 9.80 |
| ATOM | 12423 | СВ | VAL | 1860 | | -22.397 | 17.824 | 1.00 9.99 |
| ATOM | 12424 | | VAL | 1860 | | -22.674 | 19.258 | 1.00 10.58 |
| ATOM | 12425 | | VAL | 1860 | | -23.222 | 16.855 | 1.00 10.13 |
| | | | | | | | | |

| ATOM | 12426 | С | VAL | 1860 | 14.343 -20.116 | 18.507 | 1.00 9.52 |
|--------------|----------------|-----------|------------|--------------|----------------------------------|------------------|--------------------------|
| ATOM | 12427 | 0 | VAL | 1860 | 15.570 -20.165 | 18.449 | 1.00 9.57 |
| ATOM | 12428 | N | THR | 1861 | 13.691 -19.419 | 19.435 | 1.00 9.74 |
| MOTA | 12429 | CA | THR | 1861 | 14.412 -18.633 | 20.432 | 1.00 12.01 |
| MOTA | 12430 | CB | THR | 1861 | 13.845 -17.199 | 20.509 | 1.00 15.97 |
| MOTA | 12431 | OG1 | THR | 1861 | 13.816 -16.623 | 19.192 | 1.00 20.58 |
| MOTA | 12432 | CG2 | THR | 1861 | 14.722 -16.325 | 21.387 | 1.00 23.39 |
| MOTA | 12433 | С | THR | 1861 | 14.367 -19.270 | 21.822 | 1.00 11.32 |
| MOTA | 12434 | 0 | THR | 1861 | 13.603 -20.199 | 22.072 | 1.00 9.35 |
| MOTA | 12435 | N | VAL | 1862 | 15.214 -18.773 | 22.717 | 1.00 11.39 |
| MOTA | 12436 | CA | VAL | 1862 | 15.251 -19.275 | 24.079 | 1.00 11.60 |
| MOTA | 12437 | CB | VAL | 1862 | 16.309 -18.524 | 24.920 | 1.00 11.99 |
| MOTA | 12438 | CG1 | VAL | 1862 | 16.238 -18.982 | 26.367 | 1.00 13.48 |
| MOTA | 12439 | CG2 | VAL | 1862 | 17.715 -18.775 | 24.349 | 1.00 13.06 |
| MOTA | 12440 | C | VAL | 1862 | 13.864 -19.080 | 24.695 | 1.00 11.31 |
| ATOM | 12441 | 0 | VAL | 1862 | 13.366 -19.955 | 25.398 | 1.00 11.62 |
| ATOM | 12442 | N | ALA | 1863 | 13.227 -17.941 | 24.421 | 1.00 10.93 |
| ATOM | 12443 | CA | ALA | 1863 | 11.893 -17.697 | 24.966 24.535 | 1.00 10.99 1.00 13.54 |
| ATOM | 12444 | CB | ALA ALA | 1863 | 11.380 -16.336 10.925 -18.773 | 24.333 | 1.00 13.34 |
| ATOM | 12445 12446 | С | ALA | 1863 1863 | 10.925 -16.773 | 25.278 | 1.00 10.73 |
| MOTA MOTA | 12447 | O N | ASP | 1864 | 11.013 -19.141 | 23.221 | 1.00 8.92 |
| ATOM | 12447 | CA | ASP | 1864 | 10.135 -20.191 | 22.669 | 1.00 9.84 |
| ATOM | 12449 | CB | ASP | 1864 | 10.452 -20.488 | 21.191 | 1.00 9.14 |
| ATOM | 12450 | CG | ASP | 1864 | 10.169 -19.322 | 20.263 | 1.00 9.13 |
| ATOM | 12451 | OD1 | ASP | 1864 | 9.190 -18.581 | 20.490 | 1.00 11.77 |
| ATOM | 12452 | OD2 | ASP | 1864 | 10.918 -19.167 | 19.272 | 1.00 10.86 |
| ATOM | 12453 | C | ASP | 1864 | 10.328 -21.487 | 23.456 | 1.00 9.58 |
| MOTA | 12454 | ō | ASP | 1864 | 9.358 -22.134 | 23.861 | 1.00 8.41 |
| MOTA | 12455 | N | ILE | 1865 | 11.583 -21.876 | 23.660 | 1.00 8.67 |
| ATOM | 12456 | CA | ILE | 1865 | 11.879 -23.111 | 24.398 | 1.00 9.31 |
| ATOM | 12457 | CB | ILE | 1865 | 13.409 -23.355 | 24.520 | 1.00 9.33 |
| MOTA | 12458 | CG2 | ILE | 1865 | 13.668 -24.518 | 25.470 | 1.00 11.52 |
| ATOM | 12459 | CG1 | ILE | 1865 | 14.035 -23.606 | 23.134 | 1.00 9.79 |
| MOTA | 12460 | CD1 | ILE | 1865 | 13.509 -24.855 | 22.397 | 1.00 8.07 |
| MOTA | 12461 | C | ILE | 1865 | 11.285 -23.036 | 25.808 | 1.00 9.25 |
| MOTA | 12462 | 0 | ILE | 1865 | 10.661 -23.991 | 26.283 | 1.00 9.30 |
| ATOM | 12463 | N | ALA | 1866 | 11.492 -21.906 | 26.483 | 1.00 7.42 |
| MOTA | 12464 | CA | ALA | 1866 | 10.969 -21.716 | 27.843 | 1.00 5.92 |
| MOTA | 12465 | CB | ALA | 1866 | 11.352 -20.335 | 28.373 | 1.00 6.24 |
| MOTA | 12466 | С | ALA | 1866 | 9.452 -21.879 | 27.895 | 1.00 8.68 |
| ATOM | 12467 | 0 | ALA | 1866 | 8.904 -22.480 | 28.826 | 1.00 6.71 |
| ATOM | 12468 | N | TYR | 1867 | 8.768 -21.319 | 26.903 | 1.00 7.88 |
| ATOM | 12469 | CA | TYR | 1867 | 7.307 -21.421 6.799 -20.700 | 26.817 | 1.00 9.45 1.00 8.36 |
| MOTA | 12470 | CB | TYR | 1867 | 5.304 -20.839 | 25.550 25.314 | 1.00 8.36 1.00 8.40 |
| MOTA | 12471 12472 | CG CD1 | TYR TYR | 1867 1867 | 4.384 -20.257 | 26.184 | 1.00 3.40 |
| ATOM ATOM | 12472 | CE1 | TYR | 1867 | 3.010 -20.316 | 25.930 | 1.00 11.03 |
| ATOM | 12474 | CD2 | TYR | 1867 | 4.812 -21.496 | 24.187 | 1.00 9.92 |
| ATOM | 12475 | CE2 | TYR | 1867 | 3.440 -21.561 | 23.925 | 1.00 9.81 |
| ATOM | 12476 | CZ | TYR | 1867 | 2.550 -20.968 | 24.791 | 1.00 9.83 |
| ATOM | 12477 | OH | TYR | 1867 | 1.204 -20.972 | 24.502 | 1.00 13.41 |
| ATOM | 12478 | С | TYR | 1867 | 6.844 -22.874 | 26.773 | 1.00 9.90 |
| MOTA | 12479 | 0 | TYR | 1867 | 5.984 -23.308 | 27.556 | 1.00 8.93 |
| ATOM | 12480 | N | HIS | 1868 | 7.413 -23.629 | 25.843 | 1.00 7.87 |
| ATOM | 12481 | CA | HIS | 1868 | 7.025 -25.026 | 25.691 | 1.00 10.27 |
| MOTA | 12482 | СВ | HIS | 1868 | 7.557 -25.543 | 24.349 | 1.00 9.57 |
| MOTA | 12483 | CG | HIS | 1868 | 6.843 -24.939 | 23.174 | 1.00 9.11 |
| MOTA | 12484 | | HIS | 1868 | 7.194 -23.938 | 22.330 | 1.00 9.03 |
| MOTA | 12485 | | HIS | 1868 | 5.543 -25.267 | 22.852 | 1.00 8.93 |
| MOTA | 12486 | | HIS | 1868 | 5.120 -24.490 | 21.870 | 1.00 8.96 |
| MOTA | 12487 | | HIS | 1868 | 6.102 -23.674 | 21.534 | 1.00 8.75 |
| ATOM | 12488 | C | HIS | 1868 | 7.483 -25.860 | 26.874 | 1.00 10.42 |
| ATOM | 12489 | 0 | HIS | 1868 | 6.800 -26.804 8.611 -25.481 | 27.266 27.469 | 1.00 9.01 1.00 10.19 |
| ATOM | 12490 | N | THR | 1869 | | | |
| MOTA MOTA | 12491 | CA CB | THR THR | 1869 | 9.133 -26.197 10.520 -25.639 | 28.635 29.032 | 1.00 10.01 1.00 11.08 |
| ATOM | 12492 12493 | OG1 | | 1869 1869 | 11.474 -25.995 | 28.022 | 1.00 11.08 |
| ATOM | 12493 | CG2 | THR | 1869 | 10.984 -26.205 | 30.378 | 1.00 10.61 |
| ATOM | 12494 | CGZ | THR | 1869 | 8.156 -26.077 | 29.809 | 1.00 10.51 |
| ATOM | 12495 | 0 | THR | 1869 | 7.896 -27.056 | 30.501 | 1.00 9.02 |
| ATOM | 12497 | N | ALA | 1870 | 7.607 -24.884 | 30.036 | 1.00 9.46 |
| MOTA | 12498 | CA | ALA | 1870 | 6.673 -24.719 | 31.146 | 1.00 10.75 |
| ATOM | 12499 | CB | ALA | 1870 | 6.301 -23.242 | 31.331 | 1.00 11.04 |
| MOTA | 12500 | С | ALA | 1870 | 5.416 -25.553 | 30.909 | 1.00 10.58 |
| ATOM | 12501 | 0 | ALA | 1870 | 4.886 -26.180 | 31.831 | 1.00 11.31 |
| ATOM | 12502 | N | ALA | 1871 | 4.939 -25.568 | 29.672 | 1.00 9.74 |
| | | | | | | | |

| ATOM | 12503 | CA | ALA | 1871 | 3.738 -26.332 | 29.347 | 1.00 10.34 |
|--------------|----------------|---------------|------------|--------------|----------------------------------|------------------|--------------------------|
| ATOM | 12504 | CB | ALA | 1871 | 3.323 -26.056 | 27.907 | 1.00 9.64 |
| ATOM | 12505 | C | ALA | 1871 | 3.965 -27.828 | 29.559 | 1.00 10.87 |
| ATOM | 12506 | 0 | ALA | 1871 | 3.104 -28.514 | 30.116 | 1.00 11.14 |
| ATOM | 12507 | N | VAL | 1872 | 5.119 -28.333 | 29.126 | 1.00 8.50 |
| MOTA | 12508 | CA | VAL | 1872 | 5.418 -29.754 | 29.300 | 1.00 9.80 |
| ATOM | 12509 | CB | VAL | 1872 | 6.724 -30.161 | 28.569 | 1.00 8.60 |
| ATOM | 12510 | CG1 | VAL | 1872 | 7.169 -31.563 | 29.019 | 1.00 5.70 |
| ATOM | 12511 | CG2 | VAL | 1872 | 6.483 -30.174 | 27.061 | 1.00 8.96 |
| ATOM | 12512 | С | VAL | 1872 | 5.518 -30.078 | 30.788 | 1.00 10.76 |
| ATOM | 12513 | 0 | VAL | 1872 | 4.979 -31.085 | 31.245 | 1.00 11.38 |
| ATOM | 12514 | N | ARG | 1873 | 6.192 -29.221 | 31.549 | 1.00 10.87 |
| ATOM | 12515 | CA | ARG | 1873 | 6.311 -29.450 | 32.980 | 1.00 9.93 |
| MOTA | 12516 | CB | ARG | 1873 | 7.153 -28.348 | | 1.00 7.52 |
| MOTA | 12517 | CG | ARG | 1873 | 7.288 -28.505 | | 1.00 10.26 |
| MOTA | 12518 | CD | ARG | 1873 | 7.857 -29.878 | 35.567 | 1.00 12.74 |
| MOTA | 12519 | NE | ARG | 1873 | 9.289 -30.011 | | 1.00 15.69 |
| ATOM | 12520 | CZ | ARG | 1873 | 9.939 -31.172 | | 1.00 12.78 |
| MOTA | 12521 | NH1 | ARG | 1873 | 9.290 -32.304 | | 1.00 13.43 |
| MOTA | 12522 | NH2 | ARG | 1873 | 11.242 -31.205 | | 1.00 12.86 |
| MOTA | 12523 | С | ARG | 1873 | 4.924 -29.522 | | 1.00 10.69 |
| MOTA | 12524 | 0 | ARG | 1873 | 4.726 -30.310 | | 1.00 12.04 |
| MOTA | 12525 | N | ARG | 1874 | 3.968 -28.713 | | 1.00 9.73 |
| MOTA | 12526 | CA | ARG | 1874 | 2.631 -28.750 | | 1.00 10.96 |
| MOTA | 12527 | CB | ARG | 1874 | 1.736 -27.640 | | 1.00 12.21 |
| MOTA | 12528 | CG | ARG | 1874 | 2.285 -26.245 | | 1.00 15.36 |
| MOTA | 12529 | CD | ARG | 1874 | 1.230 -25.139 | | 1.00 17.99 |
| MOTA | 12530 | NE | ARG | 1874 | 1.868 -23.843 | | |
| MOTA | 12531 | \mathbf{cz} | ARG | 1874 | 2.419 -23.101 | | 1.00 19.11 |
| MOTA | 12532 | | | 1874 | 2.397 -23.517 | | 1.00 14.81 |
| MOTA | 12533 | NH2 | ARG | 1874 | 3.027 -21.961 | | 1.00 17.47 |
| ATOM | 12534 | С | ARG | 1874 | 1.970 -30.110 | | 1.00 11.41 |
| MOTA | 12535 | О | ARG | 1874 | 1.273 -30.630 | | 1.00 14.88 |
| MOTA | 12536 | N | GLY | 1875 | 2.200 -30.696 | | 1.00 11.22 |
| MOTA | 12537 | CA | GLY | 1875 | 1.606 -31.990 | | 1.00 10.19 |
| MOTA | 12538 | С | GLY | 1875 | 2.323 -33.162 | | 1.00 10.02 |
| MOTA | 12539 | 0 | GLY | 1875 | 1.708 -34.182 | | 1.00 9.60 |
| MOTA | 12540 | N | ALA | 1876 | 3.627 -33.012 | | 1.00 11.21 |
| MOTA | 12541 | CA | ALA | 1876 | 4.455 -34.071 | | 1.00 11.50 |
| MOTA | 12542 | CB | ALA | 1876 | 5.309 -34.718 | | 1.00 14.27 |
| MOTA | 12543 | C | ALA | 1876 | 5.350 -33.513 | | 1.00 12.82 |
| MOTA | 12544 | 0 | ALA | 1876 | 6.560 -33.374 | | 1.00 11.92 |
| MOTA | 12545 | N | PRO | 1877 | 4.771 -33.210 | | 1.00 14.04 |
| ATOM | 12546 | CD | PRO | 1877 | 3.375 -33.476 | | 1.00 14.97 |
| MOTA | 12547 | CA | PRO | 1877 | 5.554 -32.657 | | 1.00 15.62 |
| MOTA | 12548 | CB | PRO | 1877 | 4.491 -32.375 | | 1.00 15.70 |
| MOTA | 12549 | CG | PRO | 1877 | 3.469 -33.421 | | 1.00 18.20 |
| ATOM | 12550 | С | PRO | 1877 | 6.699 -33.510 | | 1.00 16.14 |
| ATOM | 12551 | 0 | PRO | 1877 | 7.589 -32.992 | | 1.00 18.76 |
| ATOM | 12552 | N | ASN | 1878 | 6.686 -34.801 | | 1.00 15.89 |
| ATOM | 12553 | CA | ASN | 1878 | 7.709 -35.718 | | 1.00 17.91 |
| ATOM | 12554 | CB | ASN | 1878 | 7.038 -36.936 | | 1.00 22.40 |
| ATOM | 12555 | CG | ASN | 1878 | 6.081 -36.552 | | 1.00 25.24 |
| ATOM | 12556 | | ASN | 1878 | 6.463 -35.889 | | 1.00 29.66 |
| MOTA | 12557 | | ASN | 1878 | 4.824 -36.974 | | 1.00 28.39 |
| ATOM | 12558 | C | ASN | 1878 | 8.710 -36.209 | | 1.00 17.02 |
| ATOM | 12559 | 0 | ASN | 1878 | 9.604 -36.986 | | 1.00 16.69 |
| MOTA | 12560 | N | CYS | 1879 | 8.578 -35.763 9.487 -36.238 | | 1.00 15.26 |
| ATOM | 12561 | CA | CYS | 1879 | | | 1.00 13.68 |
| ATOM | 12562 | CB | CYS | 1879 | 8.890 -35.991 | | 1.00 14.20 |
| ATOM | 12563 | SG | CYS | 1879 | 9.037 -34.260 10.865 -35.596 | | 1.00 16.39 |
| MOTA ATOM | 12564 | C | CYS | 1879 1879 | | | 1.00 13.72 |
| | 12565 | O | CYS | | 11.085 -34.604 | | 1.00 13.75 |
| MOTA | 12566 | N | LEU | 1880 | 11.802 -36.213 13.130 -35.660 | | 1.00 13.56 1.00 13.22 |
| ATOM | 12567 | CA | LEU | 1880 | | | 1.00 13.22 |
| ATOM ATOM | 12568 | CB | LEU | 1880 | 14.185 -36.740 15.583 -36.162 | 33.317 | 1.00 12.70 |
| ATOM | 12569 12570 | CG CD1 | LEU LEU | 1880 | 16.056 -35.315 | | 1.00 12.13 |
| | | | | 1880 | 16.561 -37.299 | | 1.00 14.50 |
| MOTA | 12571 | | LEU | 1880 | | | |
| ATOM ATOM | 12572 12573 | C. | LEU | 1880 | 12.925 -34.860 12.573 -35.430 | 32.259 31.231 | 1.00 11.47 1.00 12.83 |
| ATOM | 12574 | O N | LEU | 1880 | 13.124 -33.546 | | 1.00 12.83 |
| ATOM | 12574 | CA | LEU | 1881 | 12.881 -32.705 | | 1.00 10.82 |
| MOTA | 12576 | CB | LEU LEU | 1881 | 11.882 -31.600 | | 1.00 10.82 |
| MOTA | 12576 | CG. | | 1881 | 11.152 -31.600 | | 1.00 11.46 |
| MOTA | 12577 | | LEU LEU | 1881 1881 | 10.169 -29.889 | | 1.00 14.79 |
| ATOM | 12579 | | LEU | 1881 | 12.096 -29.933 | 29.599 | 1.00 14.22 |
| | 123,7 | CD2 | 0 | 1001 | 12.070 27.933 | 27.377 | 1,.10 |

| ATOM | 12580 | С | LEU | 1881 | 14.140 -32.0 | 77 30.601 | 1.00 11.03 |
|--------------|----------------|----------|------------|--------------|------------------------------|-------------|--------------------------|
| ATOM | 12581 | ō | LEU | 1881 | 14.802 -31.2 | | 1.00 13.13 |
| ATOM | 12582 | N | LEU | 1882 | 14.460 -32.4 | | 1.00 10.50 |
| ATOM | 12583 | CA | LEU | 1882 | 15.622 -31.8 | 85 28.698 | 1.00 11.79 |
| ATOM | 12584 | CB | LEU | 1882 | 16.333 -32.9 | 52 27.868 | 1.00 11.43 |
| MOTA | 12585 | CG | LEU | 1882 | 17.203 -33.9 | 73 28.607 | 1.00 15.97 |
| MOTA | 12586 | CD1 | LEU | 1882 | 16.363 -34.7 | | 1.00 17.09 |
| ATOM | 12587 | CD2 | LEU | 1882 | 17.882 -34.8 | 78 27.577 | 1.00 16.23 |
| ATOM | 12588 | С | LEU | 1882 | 15.146 -30.7 | 67 27.787 | 1.00 13.92 |
| MOTA | 12589 | 0 | LEU | 1882 | 14.172 -30.93 | 26 27.051 | 1.00 17.46 |
| ATOM | 12590 | N | ALA | 1883 | 15.808 -29.6 | 23 27.852 | 1.00 11.32 |
| ATOM | 12591 | CA | ALA | 1883 | 15.426 -28.5 | 20 26.990 | 1.00 12.45 |
| ATOM | 12592 | CB | ALA | 1883 | 14.960 -27.3 | 42 27.824 | 1.00 12.10 |
| ATOM | 12593 | С | ALA | 1883 | 16.624 -28.1 | 32 26.144 | 1.00 11.52 |
| MOTA | 12594 | 0 | ALA | 1883 | 17.748 -28.0 | | 1.00 10.54 |
| MOTA | 12595 | N | ASP | 1884 | 16.384 -27.9 | | 1.00 12.57 |
| ATOM | 12596 | CA | ASP | 1884 | 17.447 -27.5 | | 1.00 12.76 |
| MOTA | 12597 | CB | ASP | 1884 | 16.981 -27.6 | | 1.00 13.52 |
| MOTA | 12598 | CG | ASP | 1884 | 17.351 -28.9 | | 1.00 15.04 |
| MOTA | 12599 | | ASP | 1884 | 17.887 -29.8 | | 1.00 16.51 |
| MOTA | 12600 | | ASP | 1884 | 17.098 -29.0 | | 1.00 14.48 |
| MOTA | 12601 | C | ASP | 1884 | 17.785 -26.0 | | 1.00 14.66 |
| MOTA | 12602 | О | ASP | 1884 | 16.934 -25.2 | | 1.00 13.13 |
| ATOM | 12603 | N | LEU | 1885 | 19.040 -25.7 | | 1.00 12.80 |
| ATOM | 12604 | CA | LEU | 1885 | 19.449 -24.3 | | 1.00 12.01 |
| MOTA | 12605 | CB | LEU | 1885 | 20.860 -24.0 | | 1.00 11.51 |
| ATOM | 12606 | CG | LEU | 1885 | 20.951 -24.0 | | 1.00 13.75 |
| ATOM | 12607 | | LEU | 1885 | 22.335 -23.5 | | 1.00 14.19 |
| MOTA | 12608 | CD2 | | 1885 | 19.862 -23.1 | | 1.00 15.95 |
| ATOM | 12609 | C | LEU | 1885 | 19.472 -24.1 | | 1.00 10.80 1.00 11.71 |
| ATOM | 12610 | 0 | LEU | 1885 | 20.170 -24.9 18.696 -23.2 | | 1.00 10.45 |
| ATOM | 12611 | N | PRO | 1886 1886 | 17.852 -22.2 | | 1.00 10.45 |
| ATOM ATOM | 12612 12613 | CD CA | PRO PRO | 1886 | 18.606 -23.0 | | 1.00 10.23 |
| ATOM | 12614 | CB | PRO | 1886 | 17.356 -22.1 | | 1.00 11.55 |
| ATOM | 12615 | CG | PRO | 1886 | 17.457 -21.2 | | 1.00 11.59 |
| ATOM | 12616 | C | PRO | 1886 | 19.819 -22.3 | | 1.00 11.51 |
| MOTA | 12617 | 0 | PRO | 1886 | 20.825 -22.0 | | 1.00 13.04 |
| ATOM | 12618 | N | PHE | 1887 | 19.692 -22.1 | | 1.00 9.35 |
| ATOM | 12619 | CA | PHE | 1887 | 20.723 -21.5 | | 1.00 10.68 |
| ATOM | 12620 | CB | PHE | 1887 | 20.125 -21.2 | | 1.00 11.05 |
| ATOM | 12621 | CG | PHE | 1887 | 20.992 -20.3 | | 1.00 12.47 |
| ATOM | 12622 | CD1 | | 1887 | 22.251 -20.7 | | 1.00 15.73 |
| ATOM | 12623 | | PHE | 1887 | 20.546 -19.1 | 10 14.890 | 1.00 14.62 |
| ATOM | 12624 | CE1 | PHE | 1887 | 23.058 -19.9 | 75 14.057 | 1.00 15.72 |
| ATOM | 12625 | CE2 | PHE | 1887 | 21.340 -18.2 | 76 14.092 | 1.00 13.51 |
| ATOM . | 12626 | CZ | PHE | 1887 | 22.598 -18.7 | 17 13.679 | 1.00 15.84 |
| MOTA | 12627 | С | PHE | 1887 | 21.290 -20.3 | 11 18.153 | 1.00 10.86 |
| MOTA | 12628 | 0 | PHE | 1887 | 20.547 -19.4 | | 1.00 9.48 |
| MOTA | 12629 | N | MET | 1888 | 22.614 -20.2 | | 1.00 8.23 |
| MOTA | 12630 | CA | MET | 1888 | 23.337 -19.1 | | 1.00 10.91 |
| MOTA | 12631 | CB | MET | 1888 | 23.230 -17.9 | | 1.00 13.53 |
| MOTA | 12632 | CG | MET | 1888 | 24.386 -16.9 | | 1.00 15.10 |
| MOTA | 12633 | SD | MET | 1888 | 26.011 -17.5 | | 1.00 16.09 |
| MOTA | 12634 | CE | MET | 1888 | 26.079 -17.0 | | 1.00 19.82 |
| MOTA | 12635 | C | MET | 1888 | 22.920 -18.7 | | 1.00 12.89 |
| ATOM | 12636 | 0 | MET | 1888 | 23.012 -17.5 | | 1.00 13.39 |
| MOTA | 12637 | N | ALA | 1889 | 22.468 -19.7 22.079 -19.4 | | 1.00 10.65 1.00 11.53 |
| ATOM | 12638 | CA | ALA | 1889 | 20.803 -20.1 | | 1.00 11.33 |
| ATOM | 12639 | CB | ALA ALA | 1889 1889 | 23.200 -19.7 | | 1.00 12.03 |
| ATOM ATOM | 12640 12641 | ,C | ALA | 1889 | 23.200 -19.7 | | 1.00 13.56 |
| MOTA | 12642 | N | TYR | 1890 | 24.305 -20.2 | | 1.00 13.30 |
| MOTA | 12643 | CA | TYR | 1890 | 25.439 -20.6 | | 1.00 12.50 |
| ATOM | 12644 | CB | TYR | 1890 | 25.378 -22.1 | | 1.00 12.92 |
| ATOM | 12645 | CG | TYR | 1890 | 25.067 -23.0 | | 1.00 13.64 |
| ATOM | 12646 | CD1 | | 1890 | 26.089 -23.7 | | |
| ATOM | 12647 | | TYR | 1890 | 25.809 -24.5 | | 1.00 15.46 |
| ATOM | 12648 | | TYR | 1890 | 23.750 -23.2 | | 1.00 14.15 |
| MOTA | 12649 | CE2 | | 1890 | 23.456 -24.1 | | 1.00 15.84 |
| ATOM | 12650 | CZ | TYR | 1890 | 24.488 -24.7 | | 1.00 16.93 |
| MOTA | 12651 | ОН | TYR | 1890 | 24.206 -25.6 | | 1.00 19.58 |
| ATOM | 12652 | С | TYR | 1890 | 26.743 -20.2 | 87 . 23.000 | 1.00 12.88 |
| ATOM | 12653 | 0 | TYR | 1890 | 27.716 -21.0 | | 1.00 13.54 |
| ATOM | 12654 | N | ALA | 1891 | 26.741 -19.1 | | 1.00 11.98 |
| ATOM | 12655 | CA | ALA | 1891 | 27.885 -18.6 | | 1.00 13.29 |
| ATOM | 12656 | CB | ALA | 1891 | 27.472 -17.3 | 39 20.862 | 1.00 13.53 |

| MOTA | 12657 | С | ALA | 1891 | 29.100 -18.3 | 22.490 | 1.00 13.87 |
|--------------|----------------|------------|------------|--------------|--------------------------------|-----------|--------------------------|
| MOTA | 12658 | 0 | ALA | 1891 | 30.231 -18.2 | 38 22.009 | 1.00 13.32 |
| MOTA | 12659 | N | THR | 1892 | 28.850 -18.0 | | 1.00 12.24 |
| MOTA | 12660 | CA | THR | 1892 | 29.905 -17.7 | | 1.00 12.51 |
| MOTA | 12661 | CB | THR | 1892 | 30.09816.2 | | 1.00 11.96 |
| MOTA | 12662 | OG1 | THR | 1892 | 28.968 -15.78 | | 1.00 12.50 |
| MOTA | 12663 | CG2 | THR | 1892 | 30.235 -15.5 | | 1.00 13.36 |
| MOTA | 12664 | С | THR | 1892 | 29.448 -18.43 | | 1.00 13.46 |
| ATOM | 12665 | 0 | THR | 1892 | 28.252 -18.6 | | 1.00 14.08 1.00 14.40 |
| ATOM ATOM | 12666 12667 | N CD | PRO PRO | 1893 1893 | 30.393 -18.73 31.860 -18.73 | | 1.00 14.40 |
| MOTA | 12668 | CA | PRO | 1893 | 29.988 -19.3 | | 1.00 14.16 |
| ATOM | 12669 | CB | PRO | 1893 | 31.316 -19.5 | | 1.00 17.60 |
| ATOM | 12670 | CG | PRO | 1893 | 32.274 -19.78 | | 1.00 15.21 |
| ATOM | 12671 | C | PRO | 1893 | 28.992 -18.4 | | 1.00 13.95 |
| MOTA | 12672 | 0 | PRO | 1893 | 27.964 -18.93 | | 1.00 11.45 |
| MOTA | 12673 | N | GLU | 1894 | 29.273 -17.14 | 28.994 | 1.00 15.13 |
| MOTA | 12674 | CA | GLU | 1894 | 28.374 -16.23 | 24 29.681 | 1.00 15.41 |
| ATOM | 12675 | CB | GLU | 1894 | 28.946 -14.80 | 29.634 | 1.00 19.41 |
| MOTA | 12676 | CG | GLU | 1894 | 28.154 -13.78 | | 1.00 28.99 |
| MOTA | 12677 | CD | GLU | 1894 | 29.047 -12.7 | | 1.00 32.24 |
| ATOM | 12678 | OE1 | | 1894 | 29.945 -12.2 | | 1.00 34.50 |
| ATOM | 12679 | OE2 | GLU | 1894 | 28.849 -12.3 | | 1.00 37.07 |
| MOTA | 12680 | С | GLU | 1894 | 26.951 -16.20 | | 1.00 14.63 |
| MOTA | 12681 | 0 | GLU | 1894 | 25.981 -16.2 | | 1.00 14.06 |
| MOTA | 12682 | N | GLN | 1895 | 26.811 -16.30 | | 1.00 13.27 |
| MOTA | 12683 | CA | GLN | 1895 | 25.473 -16.30 | | 1.00 14.64 |
| ATOM | 12684 | CB | GLN | 1895 | 25.539 -16.12 | | 1.00 18.45 |
| ATOM | 12685 | CG | GLN | 1895 | 26.046 -14.74 | | 1.00 26.37 |
| MOTA | 12686 | CD OE1 | GLN | 1895 | 25.806 -14.44 24.660 -14.39 | | 1.00 30.60 1.00 35.03 |
| MOTA MOTA | 12687 12688 | OE1 NE2 | GLN GLN | 1895 1895 | 26.883 -14.23 | | 1.00 35.03 |
| ATOM | 12689 | C | GLN | 1895 | 24.810 -17.70 | | 1.00 33.23 |
| ATOM | 12690 | 0 | GLN | 1895 | 23.587 -17.79 | | 1.00 12.48 |
| ATOM | 12691 | N | ALA | 1896 | 25.616 -18.75 | | 1.00 11.38 |
| ATOM | 12692 | CA | ALA | 1896 | 25.085 -20.08 | | 1.00 11.76 |
| ATOM | 12693 | CB | ALA | 1896 | 26.188 -21.14 | | 1.00 11.03 |
| ATOM | 12694 | С | ALA | 1896 | 24.510 -20.13 | | 1.00 11.59 |
| ATOM | 12695 | 0 | ALA | 1896 | 23.460 -20.73 | 33 29.387 | 1.00 11.46 |
| ATOM | 12696 | N | PHE | 1897 | 25.191 -19.4 | 75 30.094 | 1.00 10.77 |
| ATOM | 12697 | CA | PHE | 1897 | 24.738 ~19.44 | 16 31.485 | 1.00 11.53 |
| ATOM | 12698 | CB | PHE | 1897 | 25.690 -18.63 | 32.390 | 1.00 9.99 |
| ATOM | 12699 | CG | PHE | 1897 | 27.119 -19.13 | | 1.00 10.28 |
| MOTA | 12700 | | PHE | 1897 | 27.439 -20.44 | | 1.00 12.24 |
| ATOM | 12701 | CD2 | | 1897 | 28.153 -18.23 | | 1.00 9.95 |
| ATOM | 12702 | | PHE | 1897 | 28.775 -20.8 | | 1.00 12.67 |
| ATOM | 12703 | CE2 | PHE | 1897 | 29.489 -18.62 29.799 -19.9 | | 1.00 11.90 |
| MOTA | 12704 | CZ | PHE | 1897 | 29.799 -19.95 23.364 -18.83 | | 1.00 13.96 1.00 11.72 |
| ATOM ATOM | 12705 12706 | C O | PHE PHE | 1897 1897 | 22.498 -19.34 | | 1.00 11.72 1.00 10.76 |
| ATOM | 12707 | N | GLU | 1898 | 23.183 -17.66 | | 1.00 10.76 |
| ATOM | 12708 | CA | GLU | 1898 | 21.924 -16.94 | | 1.00 14.41 |
| ATOM | 12709 | СВ | GLU | 1898 | 22.072 -15.59 | | 1.00 17.46 |
| ATOM | 12710 | CG | GLU | 1898 | 20.906 -14.62 | | 1.00 25.46 |
| ATOM | 12711 | CD | GLU | 1898 | 20.594 -14.63 | 8 32.284 | 1.00 28.92 |
| ATOM | 12712 | OE1 | GLU | 1898 | 21.449 -14.15 | | 1.00 31.30 |
| ATOM | 12713 | OE2 | GLU | 1898 | 19.495 -15.10 | | 1.00 34.77 |
| MOTA | 12714 | С | GLU | 1898 | 20.793 -17.69 | | 1.00 12.46 |
| MOTA | 12715 | 0 | GLU | 1898 | 19.701 -17.79 | | 1.00 11.48 |
| MOTA | 12716 | N | ASN | 1899 | 21.045 -18.22 | | 1.00 12.32 |
| MOTA | 12717 | CA | ASN | 1899 | 19.988 -18.94 | | 1.00 11.52 |
| MOTA | 12718 | CB | ASN | 1899 | 20.318 -19.06 | | 1.00 12.87 |
| ATOM | 12719 | CG OD1 | ASN | 1899 | 20.455 -17.70 | | 1.00 14.75 |
| MOTA | 12720 | | ASN ASN | 1899 1899 | 19.690 -16.77 21.405 -17.57 | | 1.00 10.94 1.00 11.61 |
| ATOM | 12721 | C | | 1899 | 19.686 -20.31 | | 1.00 11.01 |
| ATOM ATOM | 12722 12723 | 0 | asn asn | 1899 | 18.534 -20.75 | | 1.00 11.22 |
| ATOM | 12724 | N | ALA | 1900 | 20.690 -20.98 | | 1.00 10.29 |
| ATOM | 12725 | CA | ALA | 1900 | 20.430 -22.27 | | 1.00 10.23 |
| ATOM | 12726 | СВ | ALA | 1900 | 21.746 -22.92 | | 1.00 8.73 |
| ATOM | 12727 | C | ALA | 1900 | 19.543 -21.97 | | 1.00 9.37 |
| ATOM | 12728 | 0 | ALA | 1900 | 18.551 -22.64 | | 1.00 8.92 |
| MOTA | 12729 | N | ALA | 1901 | 19.908 -20.93 | | 1.00 10.46 |
| MOTA | 12730 | CA | ALA | 1901 | 19.147 -20.55 | | 1.00 9.71 |
| MOTA | 12731 | CB | ALA | 1901 | 19.748 -19.29 | | 1.00 9.98 |
| MOTA | 12732 | С | ALA | 1901 | 17.686 -20.30 | | 1.00 9.18 |
| MOTA | 12733 | 0 | ALA | 1901 | 16.783 -20.73 | 33.823 | 1.00 9.21 |

| ATOM | 12734 | N | THR | 1902 | 17.456 -19.601 32.0 | 07 1.00 9.93 |
|--|--|--|---|--|---|---|
| MOTA | 12735 | CA | THR | 1902 | 16.092 -19.293 31.5 | 88 1.00 10.15 |
| ATOM | 12736 | СВ | THR | 1902 | 16.081 -18.483 30.2 | |
| ATOM | 12737 | OG1 | THR | 1902 | 16.814 -17.268 30.4 | |
| | 12738 | CG2 | THR | 1902 | 14.647 -18.122 29.8 | |
| ATOM | | | | | | |
| MOTA | 12739 | C | THR | 1902 | 15.264 -20.549 31.4 | |
| MOTA | 12740 | 0 | THR | 1902 | 14.156 -20.659 31.9 | |
| MOTA | 12741 | N | VAL | 1903 | 15.801 -21.506 30.6 | 55 1.00 10.07 |
| ATOM | 12742 | CA | VAL | 1903 | 15.052 -22.723 30.4 | 10 1.00 12.02 |
| ATOM | 12743 | CB | VAL | 1903 | 15.620 -23.470 29.1 | 68 1.00 13.59 |
| ATOM | 12744 | CG1 | VAL | 1903 | 16.916 -24.192 29.4 | 94 1.00 12.92 |
| ATOM | 12745 | CG2 | VAL | 1903 | 14.577 -24.403 28.6 | |
| ATOM | 12746 | c | VAL | 1903 | 14.936 -23.627 31.6 | |
| ATOM | 12747 | o | VAL | 1903 | 13.961 -24.369 31.7 | |
| | | N | MET | 1903 | 15.901 -24.509 31.7 | |
| ATOM | 12748 | | | | | |
| MOTA | 12749 | CA | MET | 1904 | 15.842 -24.351 33.7 | |
| MOTA | 12750 | CB | MET | 1904 | 17.223 -24.428 34.4 | |
| MOTA | 12751 | CG | MET | 1904 | 18.307 -25.051 33.5 | |
| MOTA | 12752 | SD | MET | 1904 | 18.226 -26.845 33.6 | 11 1.00 19.52 |
| ATOM | 12753 | CE | MET | 1904 | 18.566 -27.204 35.4 | 06 1.00 18.10 |
| ATOM | 12754 | С | MET | 1904 | 14.826 -23.742 34.7 | 61 1.00 9.98 |
| ATOM | 12755 | 0 | MET | 1904 | 14.108 -24.479 35.4 | 33 1.00 11.43 |
| ATOM | 12756 | N | ARG | 1905 | 14.770 -22.412 34.8 | |
| ATOM | 12757 | CA | ARG | 1905 | 13.799 -21.809 35.7 | |
| ATOM | 12758 | СВ | ARG | 1905 | 13.982 -20.295 35.9 | |
| ATOM | 12759 | CG | ARG | 1905 | 15.331 -19.885 36.4 | |
| ATOM | | | | 1905 | | |
| | 12760 | CD | ARG | | | |
| ATOM | 12761 | NE | ARG | 1905 | 16.652 -17.990 37.2 | |
| ATOM | 12762 | CZ | ARG | 1905 | 17.447 -17.418 36.3 | |
| ATOM | 12763 | NH1 | ARG | 1905 | 17.029 -17.233 35.1 | |
| MOTA | 12764 | NH2 | ARG | 1905 | 18.677 -17.063 36.7 | |
| MOTA | 12765 | С | ARG | 1905 | 12.398 -22.099 35.2 | |
| MOTA | 12766 | 0 | ARG | 1905 | 11.445 -22.195 36.0 | 24 1.00 10.47 |
| MOTA | 12767 | N | ALA | 1906 | 12.291 -22.274 33.9 | 46 1.00 8.58 |
| MOTA | 12768 | CA | ALA | 1906 | 11.011 -22.538 33.3 | 17 1.00 8.67 |
| ATOM | 12769 | CB | ALA | 1906 | 11.100 -22.235 31.8 | 14 1.00 9.41 |
| ATOM | 12770 | C | ALA | 1906 | 10.511 -23.963 33.5 | |
| ATOM | 12771 | ō | ALA | 1906 | 9.351 -24.270 33.2 | |
| ATOM | 12772 | N | GLY | 1907 | 11.382 -24.841 34.0 | |
| ATOM | 12773 | CA | GLY | 1907 | 10.962 -26.209 34.2 | |
| | | | | | | |
| MOTA | 12774 | C | GLY | 1907 | 11.889 -27.330 33.8 | |
| ATOM | 12775 | 0 | GLY | 1907 | 11.684 -28.485 34.2 | |
| ATOM | 12776 | N | ALA | 1908 | 12.907 -27.009 33.0 | |
| MOTA | 12777 | CA | ALA | 1908 | 13.851 -28.026 32.6 | |
| MOTA | 12778 | CB | ALA | 1908 | 14.702 -27.455 31.4 | |
| MOTA | 12779 | С | ALA | 1908 | 14.758 -28.529 33.7 | |
| MOTA | 40000 | _ | | | | 39 1.00 11.38 |
| | 12780 | 0 | ALA | 1908 | 14.955 -27.848 34.7 | |
| ATOM | 12780 | | ALA ASN | 1908 1909 | 14.955 -27.848 34.7 15.303 -29.729 33.5 | 47 1.00 8.45 |
| ATOM ATOM | | .0 | | | | 47 1.00 8.45 57 1.00 11.47 |
| MOTA | 12781 12782 | O N CA | ASN ASN | 1909 1909 | 15.303 -29.729 33.5 16.205 -30.302 34.5 | 17 1.00 8.45 57 1.00 11.47 54 1.00 10.53 |
| ATOM ATOM | 12781 12782 12783 | N CA CB | ASN ASN ASN | 1909 1909 1909 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 | 47 1.00 8.45 57 1.00 11.47 64 1.00 10.53 39 1.00 12.92 |
| MOTA MOTA MOTA | 12781 12782 12783 12784 | O N CA CB CG | ASN ASN ASN ASN | 1909 1909 1909 1909 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 | 47 1.00 8.45 57 1.00 11.47 64 1.00 10.53 39 1.00 12.92 56 1.00 14.93 |
| ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 | N CA CB CG OD1 | ASN ASN ASN ASN ASN | 1909 1909 1909 1909 1909 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 | 47 1.00 8.45 57 1.00 11.47 54 1.00 10.53 39 1.00 12.92 56 1.00 14.93 39 1.00 14.28 |
| ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 | O N CA CB CG OD1 ND2 | ASN ASN ASN ASN ASN | 1909 1909 1909 1909 1909 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 | 47 1.00 8.45 57 1.00 11.47 64 1.00 10.53 89 1.00 12.92 66 1.00 14.93 89 1.00 14.28 28 1.00 10.46 |
| ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 | O N CA CB CG OD1 ND2 C | ASN ASN ASN ASN ASN ASN | 1909 1909 1909 1909 1909 1909 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 | 47 1.00 8.45 57 1.00 11.47 54 1.00 10.53 9 1.00 12.92 1.00 14.93 1.00 14.28 1.00 10.46 1.00 11.82 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 | N CA CB CG OD1 ND2 C | ASN ASN ASN ASN ASN ASN ASN | 1909 1909 1909 1909 1909 1909 1909 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 | 47 1.00 8.45 57 1.00 11.47 54 1.00 10.53 39 1.00 12.92 56 1.00 14.93 39 1.00 14.28 28 1.00 10.46 70 1.00 11.82 32 1.00 12.44 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12789 | N CA CB CG OD1 ND2 C O | ASN ASN ASN ASN ASN ASN ASN MET | 1909 1909 1909 1909 1909 1909 1909 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 | 47 1.00 8.45 57 1.00 11.47 64 1.00 10.53 39 1.00 12.92 1.00 14.93 39 1.00 14.28 28 1.00 10.46 70 1.00 11.82 32 1.00 12.44 53 1.00 10.66 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12789 12790 | O N CA CB CG OD1 ND2 C O N CA | ASN ASN ASN ASN ASN ASN ASN MET MET | 1909 1909 1909 1909 1909 1909 1909 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 | 47 1.00 8.45 57 1.00 11.47 54 1.00 10.53 39 1.00 12.92 56 1.00 14.93 30 1.00 14.28 28 1.00 10.46 70 1.00 11.82 32 1.00 12.44 53 1.00 10.66 50 1.00 11.23 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12789 12790 12791 | O N CA CB CG OD1 ND2 C O N CA CB | ASN ASN ASN ASN ASN ASN ASN MET MET MET | 1909 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 | 47 1.00 8.45 57 1.00 11.47 64 1.00 10.53 39 1.00 12.92 56 1.00 14.28 28 1.00 10.46 70 1.00 12.44 53 1.00 10.66 50 1.00 11.23 99 1.00 11.33 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12789 12790 12791 12792 | O N CA CB OD1 ND2 C O N CA CB CG | ASN ASN ASN ASN ASN ASN MET MET MET MET | 1909 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 | 47 1.00 8.45 57 1.00 11.47 54 1.00 10.53 39 1.00 12.92 56 1.00 14.93 39 1.00 10.46 70 1.00 11.82 32 1.00 10.46 70 1.00 11.82 32 1.00 10.66 50 1.00 11.23 39 1.00 11.33 50 1.00 15.81 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12789 12790 12791 | O N CA CB OD1 ND2 C O N CA CB CG SD | ASN ASN ASN ASN ASN ASN ASN MET MET MET | 1909 1909 1909 1909 1909 1909 1909 1910 1910 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 | 47 1.00 8.45 57 1.00 11.47 54 1.00 10.53 9 1.00 12.92 1.00 14.93 1.00 10.46 1.00 10.46 1.00 11.82 1.00 10.46 1.00 10.66 1.00 11.23 1.00 10.66 1.00 11.23 1.00 15.81 1.00 17.80 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12789 12790 12791 12792 | O N CA CB OD1 ND2 C O N CA CB CG | ASN ASN ASN ASN ASN ASN MET MET MET MET | 1909 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 | 47 1.00 8.45 57 1.00 11.47 54 1.00 10.53 9 1.00 12.92 1.00 14.93 1.00 10.46 1.00 10.46 1.00 11.82 1.00 10.46 1.00 10.66 1.00 11.23 1.00 10.66 1.00 11.23 1.00 15.81 1.00 17.80 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12789 12790 12791 12792 12793 | O N CA CB OD1 ND2 C O N CA CB CG SD | ASN ASN ASN ASN ASN ASN MET MET MET MET MET | 1909 1909 1909 1909 1909 1909 1909 1910 1910 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 | 47 1.00 8.45 57 1.00 11.47 54 1.00 10.53 39 1.00 12.92 56 1.00 14.93 39 1.00 14.28 28 1.00 10.46 70 1.00 11.82 32 1.00 12.44 53 1.00 10.66 1.00 11.23 99 1.00 11.33 50 1.00 15.81 27 1.00 17.80 27 1.00 18.58 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12789 12790 12791 12792 12793 12794 | O N CA CB OD1 ND2 C O N CA CB CG SD CE | ASN ASN ASN ASN ASN ASN ASN MET MET MET MET MET MET | 1909 1909 1909 1909 1909 1909 1909 1910 1910 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 21.887 -34.311 32.0 | 47 1.00 8.45 57 1.00 11.47 54 1.00 10.53 39 1.00 12.92 50 1.00 14.28 28 1.00 10.46 70 1.00 11.82 32 1.00 12.44 53 1.00 10.66 50 1.00 11.23 90 1.00 15.81 27 1.00 15.81 27 1.00 18.58 21 1.00 10.32 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12789 12790 12791 12792 12793 12794 12795 12796 | O N CA CB CG ON CA CB CG SD CE C O | ASN ASN ASN ASN ASN ASN ASN MET MET MET MET MET MET MET MET MET | 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 21.887 -34.311 32.0 18.822 -29.716 30.6 17.730 -29.632 30.0 | 47 1.00 8.45 57 1.00 11.47 64 1.00 10.53 39 1.00 12.92 56 1.00 14.28 28 1.00 10.46 70 1.00 11.82 28 1.00 10.46 70 1.00 11.82 39 1.00 10.66 50 1.00 11.33 50 1.00 15.81 1.00 17.80 27 1.00 17.80 27 1.00 18.58 28 1.00 10.64 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12789 12790 12791 12792 12793 12794 12795 | O N CA CB OD1 ND2 C O N CA CB CG SD CE C | ASN ASN ASN ASN ASN ASN ASN MET MET MET MET MET MET MET | 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 21.887 -34.311 32.0 18.822 -29.716 30.6 17.730 -29.632 30.0 | 47 1.00 8.45 57 1.00 11.47 1.00 10.53 39 1.00 12.92 56 1.00 14.93 39 1.00 14.28 28 1.00 10.46 70 1.00 11.82 32 1.00 12.44 33 1.00 10.66 50 1.00 11.23 99 1.00 11.33 50 1.00 15.81 27 1.00 17.80 27 1.00 18.58 27 1.00 10.32 36 1.00 10.64 36 1.00 9.77 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12786 12787 12788 12789 12790 12791 12792 12793 12794 12795 12796 12797 12798 | O N CA CB CG OD 1 CA CB CG SC C C O N CA CC | ASN ASN ASN ASN ASN ASN MET MET MET MET MET MET MET MET MET VAL VAL | 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 21.887 -34.311 32.0 18.822 -29.716 30.6 17.730 -29.632 30.0 19.941 -29.223 30.0 19.942 -28.561 28.7 | 47 1.00 8.45 57 1.00 11.47 1.00 10.53 39 1.00 12.92 56 1.00 14.93 39 1.00 14.28 28 1.00 10.46 70 1.00 11.82 32 1.00 12.44 50 1.00 10.66 50 1.00 11.23 50 1.00 15.81 27 1.00 18.58 27 1.00 18.58 27 1.00 10.32 36 1.00 10.32 36 1.00 9.77 91 1.00 10.49 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12790 12791 12792 12793 12794 12795 12796 12797 12798 12799 | O N CA CB CG SD CC O N CA CB CC | ASN ASN ASN ASN ASN ASN MET MET MET MET MET MET MET MET VAL VAL VAL | 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 21.887 -34.311 32.0 18.822 -29.716 30.6 17.730 -29.632 30.0 19.941 -29.223 30.0 19.942 -28.561 28.7 20.552 -27.149 28.9 | 47 1.00 8.45 57 1.00 11.47 54 1.00 10.53 1.00 12.92 56 1.00 14.93 39 1.00 12.46 70 1.00 11.82 32 1.00 12.44 53 1.00 10.66 50 1.00 11.23 99 1.00 11.33 50 1.00 15.81 27 1.00 17.80 27 1.00 18.58 1.00 10.64 1.00 10.64 1.00 10.64 1.00 10.64 1.00 10.64 1.00 10.64 1.00 10.64 1.00 10.49 1.00 10.49 1.00 14.32 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12790 12791 12792 12793 12794 12795 12796 12797 12798 12799 12799 | O N CA CB CG SD CE C O N CA CB CG | ASN ASN ASN ASN ASN ASN MET MET MET MET MET MET MET VAL VAL VAL | 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 21.887 -34.311 32.0 18.822 -29.716 30.6 17.730 -29.632 30.0 19.941 -29.223 30.0 19.942 -28.561 28.7 20.552 -27.149 28.9 20.525 -26.477 27.5 | 47 1.00 8.45 57 1.00 11.47 54 1.00 10.53 1.00 12.92 1.00 14.93 39 1.00 14.28 28 1.00 10.46 70 1.00 11.82 32 1.00 12.44 53 1.00 10.66 50 1.00 11.23 99 1.00 11.33 50 1.00 15.81 27 1.00 17.80 27 1.00 18.58 1.00 10.64 1.00 10.64 1.00 10.64 1.00 10.64 1.00 10.64 1.00 10.64 1.00 10.64 1.00 10.64 1.00 10.49 1.00 14.32 1.00 10.49 1.00 14.32 1.00 10.49 1.00 10.49 1.00 10.49 1.00 10.49 1.00 10.49 1.00 10.49 1.00 10.49 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12790 12791 12792 12793 12794 12795 12796 12797 12798 12799 12800 12801 | O N CA CB CG SD CE C O N CA CB CG | ASN ASN ASN ASN ASN ASN MET MET MET MET MET MET VAL VAL VAL VAL | 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 21.887 -34.311 32.0 18.822 -29.716 30.6 17.730 -29.632 30.0 19.941 -29.223 30.0 19.941 -29.223 30.0 19.942 -28.561 28.7 20.552 -27.149 28.9 20.525 -26.477 27.5 19.784 -26.322 29.9 | 47 1.00 8.45 57 1.00 11.47 64 1.00 10.53 69 1.00 12.92 66 1.00 14.28 88 1.00 10.46 70 1.00 11.82 88 1.00 10.66 60 1.00 11.23 99 1.00 11.33 60 1.00 15.81 27 1.00 18.58 27 1.00 18.58 27 1.00 10.64 86 1.00 9.77 91 1.00 10.49 91 1.00 10.49 91 1.00 10.49 91 1.00 10.49 91 1.00 10.49 91 1.00 10.49 91 1.00 10.49 91 1.00 10.49 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12790 12791 12792 12793 12794 12795 12796 12797 12798 12799 12800 12801 12802 | O N CA CB CG SD C C C C C C C C C C C C C C C C C C | ASN ASN ASN ASN ASN ASN ASN MET MET MET MET MET MET VAL VAL VAL VAL VAL | 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 21.887 -34.311 32.0 18.822 -29.716 30.6 17.730 -29.632 30.0 19.941 -29.223 30.0 19.942 -28.561 28.7 20.552 -27.149 28.9 20.5552 -26.477 27.5 19.784 -26.322 29.9 20.752 -29.368 27.7 | 47 1.00 8.45 67 1.00 11.47 64 1.00 10.53 89 1.00 12.92 66 1.00 14.28 28 1.00 10.46 70 1.00 11.82 32 1.00 12.44 650 1.00 11.23 99 1.00 11.33 60 1.00 15.81 27 1.00 17.80 27 1.00 18.58 20 1.00 10.64 86 1.00 9.77 91 1.00 10.49 104 1.00 10.49 104 1.00 10.49 105 10.00 10.49 106 10.00 10.49 107 100 10.49 100 10.49 100 10.49 100 10.49 100 10.49 100 10.49 100 10.49 100 10.49 100 10.49 100 10.49 100 10.49 100 10.49 100 10.49 100 10.49 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12789 12790 12791 12792 12793 12794 12795 12796 12797 12798 12799 12800 12800 12802 12803 | O N CA CB CG SD CE C O N CA CB CG CC O N CA CB CG CC O N CA CB CG CC C O CC CC C C C C C C C C C C C C | ASN ASN ASN ASN ASN ASN MET MET MET MET MET VAL VAL VAL VAL VAL VAL | 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 21.887 -34.311 32.0 18.822 -29.716 30.6 17.730 -29.632 30.0 19.941 -29.223 30.0 19.941 -29.223 30.0 19.942 -28.561 28.7 20.552 -27.149 28.9 20.525 -26.477 27.5 19.784 -26.322 29.9 20.752 -29.368 27.7 21.758 -29.989 28.1 | 47 1.00 8.45 67 1.00 11.47 64 1.00 10.53 89 1.00 12.92 66 1.00 14.93 89 1.00 10.46 70 1.00 11.82 82 1.00 12.44 83 1.00 10.66 650 1.00 11.23 99 1.00 15.81 27 1.00 18.58 90 1.00 10.32 80 1.00 10.46 81 1.00 10.32 81 1.00 10.32 81 1.00 10.32 81 1.00 10.32 81 1.00 10.32 81 1.00 10.32 81 1.00 10.32 81 1.00 10.32 81 1.00 10.32 81 1.00 10.49 81 1.00 10.49 81 1.00 10.49 81 1.00 10.29 82 1.00 11.18 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12786 12787 12788 12789 12790 12791 12792 12793 12794 12795 12796 12799 12800 12801 12801 12802 12803 12804 | O N CA CB CG SD CE C O N CA CB CG1 CG2 C O N | ASN ASN ASN ASN ASN ASN MET MET MET MET MET VAL VAL VAL VAL VAL VAL LYS | 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 21.887 -34.311 32.0 18.822 -29.716 30.6 17.730 -29.632 30.0 19.941 -29.223 30.0 19.942 -28.561 28.7 20.552 -27.149 28.9 20.525 -26.477 27.5 19.784 -26.322 29.9 20.752 -29.368 27.7 21.758 -29.989 28.1 20.304 -29.364 26.5 | 47 1.00 8.45 67 1.00 11.47 64 1.00 10.53 1.00 12.92 66 1.00 14.93 89 1.00 12.42 81 1.00 10.46 70 1.00 11.82 82 1.00 12.44 650 1.00 11.23 99 1.00 11.23 99 1.00 15.81 27 1.00 18.58 100 10.32 1.00 10.32 1.00 10.46 1.00 9.77 1.00 10.49 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12790 12791 12792 12793 12794 12795 12796 12797 12798 12799 12800 12801 12801 12802 12803 12804 12805 | O N CA CB CG SD CE C O N CA CB CG1 CG2 C O N CA CB | ASN ASN ASN ASN ASN ASN MET MET MET MET MET VAL VAL VAL VAL VAL VAL VAL LYS LYS | 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 21.887 -34.311 32.0 18.822 -29.716 30.6 17.730 -29.632 30.0 19.941 -29.223 30.0 19.942 -28.561 28.7 20.552 -27.149 28.9 20.555 -26.477 27.5 19.784 -26.322 29.9 20.752 -29.368 27.7 21.758 -29.989 28.1 20.304 -29.364 26.5 21.019 -30.062 25.4 | 47 1.00 8.45 67 1.00 11.47 64 1.00 10.53 1.00 12.92 66 1.00 14.93 88 1.00 10.46 70 1.00 11.82 82 1.00 12.44 63 1.00 10.66 65 1.00 11.23 69 1.00 15.81 60 1.00 15.81 60 1.00 10.32 7 1.00 18.58 61 1.00 10.64 63 1.00 10.64 64 1.00 9.77 61 1.00 10.49 64 1.00 14.32 65 1.00 10.49 65 1.00 10.49 66 1.00 9.77 67 1.00 10.49 68 1.00 10.49 69 1.00 11.18 60 1.00 12.97 61 1.00 12.97 61 1.00 11.26 63 1.00 11.63 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12790 12791 12792 12793 12794 12795 12796 12797 12798 12799 12800 12801 12802 12803 12803 12805 12806 | O N CA CB CG CG CCA CCB CGC CCA CCB CCC CCA CCB CCCC CCA CCCCCC CCA CCCCCCCC | ASN ASN ASN ASN ASN ASN MET MET MET MET MET VAL VAL VAL VAL VAL VAL LYS LYS | 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 21.887 -34.311 32.0 18.822 -29.716 30.6 17.730 -29.632 30.0 19.941 -29.223 30.0 19.942 -28.561 28.7 20.552 -27.149 28.9 20.555 -26.477 27.5 19.784 -26.322 29.9 20.752 -29.368 27.7 21.758 -29.989 28.1 20.304 -29.364 26.5 21.019 -30.062 25.4 20.088 -30.999 24.7 | 47 1.00 8.45 67 1.00 11.47 64 1.00 10.53 1.00 12.92 66 1.00 14.93 89 1.00 12.44 67 1.00 10.66 67 1.00 11.82 81 1.00 10.66 67 1.00 11.33 89 1.00 17.80 80 1.00 15.81 80 1.00 10.32 80 1.00 10.32 80 1.00 10.32 80 1.00 10.32 80 1.00 10.32 80 1.00 10.32 80 1.00 10.32 80 1.00 10.32 80 1.00 10.64 81 1.00 10.64 82 1.00 10.64 83 1.00 10.64 84 1.00 10.64 85 1.00 10.64 86 1.00 10.64 87 1.00 10.64 88 1.00 10.64 89 1.00 10.64 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12786 12787 12788 12799 12790 12791 12792 12793 12794 12795 12796 12797 12798 12799 12800 12801 12802 12803 12804 12805 12806 12807 | O N CA CB CG CC C O N CA CB CG CC C C C C C C C C C C C C C C C | ASN ASN ASN ASN ASN ASN MET MET MET MET MET VAL VAL VAL VAL VAL LYS LYS LYS | 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 21.887 -34.311 32.0 18.822 -29.716 30.6 17.730 -29.632 30.0 19.941 -29.223 30.0 19.942 -28.561 28.7 20.552 -27.149 28.9 20.555 -26.477 27.5 19.784 -26.322 29.9 20.752 -29.368 27.7 21.758 -29.989 28.1 20.304 -29.364 26.5 21.019 -30.062 25.4 20.088 -30.999 24.7 20.806 -31.774 23.5 | 47 1.00 8.45 67 1.00 11.47 64 1.00 10.53 89 1.00 12.92 66 1.00 14.28 88 1.00 10.46 70 1.00 11.82 89 1.00 12.44 653 1.00 10.66 650 1.00 11.23 99 1.00 15.81 807 1.00 15.81 807 1.00 15.81 807 1.00 15.81 807 1.00 10.32 808 1.00 10.64 809 1.00 10.32 809 1.00 10.32 809 1.00 10.32 809 1.00 10.49 809 1.00 10.49 809 1.00 11.18 809 1.00 10.49 809 1.00 11.26 809 1.00 11.26 809 1.00 11.26 809 1.00 11.26 809 1.00 11.26 809 1.00 11.26 809 1.00 11.26 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12790 12791 12792 12793 12794 12795 12796 12797 12798 12799 12800 12801 12802 12803 12803 12805 12806 | O N CA CB CG CG CCA CCB CGC CCA CCB CCC CCA CCB CCCC CCA CCCCCC CCA CCCCCCCC | ASN ASN ASN ASN ASN ASN MET MET MET MET MET VAL VAL VAL VAL VAL VAL LYS LYS | 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 21.887 -34.311 32.0 18.822 -29.716 30.6 17.730 -29.632 30.0 19.941 -29.223 30.0 19.941 -29.223 30.0 19.942 -28.561 28.7 20.555 -26.477 27.5 19.784 -26.322 29.9 20.752 -29.368 27.7 21.758 -29.989 28.1 20.304 -29.364 26.5 21.019 -30.062 25.4 20.088 -30.999 24.7 20.806 -31.774 23.5 20.027 -33.015 23.1 | 47 1.00 8.45 67 1.00 11.47 64 1.00 10.53 89 1.00 12.92 66 1.00 14.93 89 1.00 12.92 80 1.00 10.46 70 1.00 11.82 81 1.00 10.66 650 1.00 11.23 89 1.00 15.81 80 1.00 15.81 80 1.00 15.81 80 1.00 10.32 81 1.00 10.32 81 1.00 10.32 81 1.00 10.32 81 1.00 10.49 81 1.00 10.49 81 1.00 10.49 81 1.00 12.97 82 1.00 11.18 82 1.00 12.97 83 1.00 11.26 84 1.00 12.97 85 1.00 11.63 86 1.00 11.63 87 1.00 11.63 88 1.00 12.97 89 1.00 11.63 80 1.00 11.63 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12786 12787 12788 12799 12790 12791 12792 12793 12794 12795 12796 12797 12798 12799 12800 12801 12802 12803 12804 12805 12806 12807 | O N CA CB CG SD C CE C O N CA CB CG1 CG2 C O N CA CB CG1 CG2 C C C C C C C C C C C C C C C C C C | ASN ASN ASN ASN ASN ASN MET MET MET MET MET VAL VAL VAL VAL VAL LYS LYS LYS | 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 21.887 -34.311 32.0 18.822 -29.716 30.6 17.730 -29.632 30.0 19.941 -29.223 30.0 19.942 -28.561 28.7 20.552 -27.149 28.9 20.555 -26.477 27.5 19.784 -26.322 29.9 20.752 -29.368 27.7 21.758 -29.989 28.1 20.304 -29.364 26.5 21.019 -30.062 25.4 20.088 -30.999 24.7 20.806 -31.774 23.5 | 47 1.00 8.45 67 1.00 11.47 64 1.00 10.53 89 1.00 12.92 66 1.00 14.93 89 1.00 12.92 80 1.00 10.46 70 1.00 11.82 81 1.00 10.66 650 1.00 11.23 89 1.00 15.81 80 1.00 15.81 80 1.00 15.81 80 1.00 10.32 81 1.00 10.32 81 1.00 10.32 81 1.00 10.32 81 1.00 10.49 81 1.00 10.49 81 1.00 10.49 81 1.00 12.97 82 1.00 11.18 82 1.00 12.97 83 1.00 11.26 84 1.00 12.97 85 1.00 11.63 86 1.00 11.63 87 1.00 11.63 88 1.00 12.97 89 1.00 11.63 80 1.00 11.63 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 12781 12782 12783 12784 12785 12786 12787 12788 12799 12791 12792 12793 12794 12795 12796 12797 12798 12799 12800 12801 12802 12803 12804 12805 12807 12807 | O N CA CB CG SD C C O N CA CB CG CC C O N CA CB CG CC C C C C C C C C C C C C C C C | ASN ASN ASN ASN ASN ASN ASN MET MET MET MET VAL VAL VAL VAL VAL LYS LYS LYS LYS | 1909 1909 1909 1909 1909 1909 1910 1910 | 15.303 -29.729 33.5 16.205 -30.302 34.5 15.804 -31.727 34.9 14.432 -31.812 35.5 14.140 -31.192 36.5 13.577 -32.595 34.9 17.593 -30.385 33.9 18.569 -30.560 34.6 17.670 -30.262 32.6 18.934 -30.391 31.9 19.228 -31.888 31.7 20.340 -32.264 30.8 20.549 -34.076 30.8 21.887 -34.311 32.0 18.822 -29.716 30.6 17.730 -29.632 30.0 19.941 -29.223 30.0 19.941 -29.223 30.0 19.942 -28.561 28.7 20.555 -26.477 27.5 19.784 -26.322 29.9 20.752 -29.368 27.7 21.758 -29.989 28.1 20.304 -29.364 26.5 21.019 -30.062 25.4 20.088 -30.999 24.7 20.806 -31.774 23.5 20.027 -33.015 23.1 | 47 1.00 8.45 67 1.00 11.47 64 1.00 10.53 83 1.00 12.92 66 1.00 14.93 89 1.00 12.92 88 1.00 10.46 70 1.00 11.82 82 1.00 12.44 83 1.00 10.66 850 1.00 11.23 850 1.00 15.81 87 1.00 18.58 87 1.00 17.80 87 1.00 18.58 87 1.00 10.32 88 1.00 10.49 91 1.00 10.49 91 1.00 10.49 91 1.00 10.49 91 1.00 12.97 91 1.00 12.97 92 1.00 11.18 92 1.00 11.18 93 1.00 12.97 94 1.00 12.97 95 1.00 11.63 96 1.00 11.63 97 1.00 11.64 98 1.00 12.97 98 1.00 11.69 |

| ATOM | 12811 | С | LYS | 1912 | 21.607 | -29.027 | 24.522 | 1.00 10.56 |
|--------------|----------------|-----------|------------|--------------|--------|--------------------|------------------|--------------------------|
| MOTA | 12812 | 0 | LYS | 1912 | 20.928 | -28.077 | 24.128 | 1.00 12.27 |
| MOTA | 12813 | N | ILE | 1913 | 22.875 | -29.208 | 24.169 | 1.00 11.16 |
| ATOM | 12814 | CA | ILE | 1913 | 23.566 | -28.301 | 23.260 | 1.00 14.22 |
| MOTA | 12815 | CB | ILE | 1913 | 24.541 | -27.375 | 24.034 | 1.00 16.27 |
| MOTA | 12816 | CG2 | ILE | 1913 | | -26.374 | 24.883 | 1.00 15.84 |
| MOTA | 12817 | CG1 | ILE | 1913 | | -28.206 | 24.925 | 1.00 18.46 |
| MOTA | 12818 | CD1 | ILE | 1913 | | -27.376 | 25.786 | 1.00 18.67 |
| MOTA | 12819 | С | ILE | 1913 | | -29.121 | 22.228 | 1.00 15.17 |
| MOTA | 12820 | 0 | ILE | 1913 | | -30.149 | 22.563 | 1.00 15.09 |
| ATOM | 12821 | N | GLU | 1914 | | -28.671 | 20.975 | 1.00 15.40 |
| MOTA | 12822 | CA | GLU | 1914 | | -29.392 | 19.889 | 1.00 16.44 |
| ATOM | 12823 | CB | GLU | 1914 | | -29.272 | 18.582 | 1.00 19.74 |
| ATOM | 12824 | CG | GLU | 1914 | | -29.426 | 18.725 | 1.00 25.29 |
| ATOM | 12825 | CD | GLU | 1914 | | -29.391 | 17.387 | 1.00 28.05 1.00 28.95 |
| MOTA | 12826 12827 | | GLU GLU | 1914 1914 | | -28.626 -30.120 | 16.497 17.231 | 1.00 28.93 |
| ATOM ATOM | 12828 | C | GLU | 1914 | | -28.893 | 19.623 | 1.00 15.88 |
| ATOM | 12829 | .0 | GLU | 1914 | | -27.696 | 19.463 | 1.00 14.70 |
| MOTA | 12830 | N | GLY | 1915 | | -29.805 | 19.550 | 1.00 16.86 |
| ATOM | 12831 | CA | GLY | 1915 | | -29.379 | 19.288 | 1.00 18.17 |
| ATOM | 12832 | C | GLY | 1915 | | -30.355 | 19.788 | 1.00 20.08 |
| MOTA | 12833 | ō | GLY | 1915 | | -31.203 | 20.631 | 1.00 21.39 |
| ATOM | 12834 | N | GLY | 1916 | 30.999 | | 19.264 | 1.00 20.87 |
| ATOM | 12835 | CA | GLY | 1916 | 32.086 | -31.091 | 19.662 | 1.00 22.00 |
| MOTA | 12836 | С | GLY | 1916 | 32.949 | -30.518 | 20.768 | 1.00 22.33 |
| MOTA | 12837 | 0 | GLY | 1916 | 32.449 | -29.886 | 21.705 | 1.00 21.23 |
| ATOM | 12838 | N | GLU | 1917 | 34.258 | -30.720 | 20.656 | 1.00 22.96 |
| MOTA | 12839 | CA | GLU | 1917 | 35.178 | -30.232 | 21.677 | 1.00 22.46 |
| MOTA | 12840 | CB | GLU | 1917 | | -30.681 | 21.376 | 1.00 26.72 |
| ATOM | 12841 | CG | GLU | 1917 | | -32.014 | 22.003 | 1.00 33.75 |
| MOTA | 12842 | CD | GLU | 1917 | | -32.087 | 22.494 | 1.00 34.57 |
| ATOM | 12843 | | GLU | 1917 | | -31.190 | 23.257 | 1.00 37.45 |
| ATOM | 12844 | | GLU | 1917 | | -33.048 | 22.120 | 1.00 39.06 |
| ATOM | 12845 | C | GLU | 1917 | 35.189 | | 21.944 | 1.00 19.95 |
| ATOM | 12846 | 0 | GLU | 1917 | | -28.324 | 23.018 | 1.00 18.13 |
| ATOM | 12847 | N | TRP | 1918 | | -27.920 -26.492 | 20.994 21.255 | 1.00 18.83 1.00 16.44 |
| ATOM ATOM | 12848 12849 | CA CB | TRP TRP | 1918 1918 | | -25.680 | 20.010 | 1.00 16.44 |
| ATOM | 12850 | CG | TRP | 1918 | | -25.705 | 19.630 | 1.00 15.75 |
| ATOM | 12851 | CD2 | | 1918 | | -24.702 | 19.927 | 1.00 15.75 |
| ATOM | 12852 | | TRP | 1918 | 30.728 | -25.106 | 19.323 | 1.00 16.90 |
| ATOM | 12853 | CE3 | TRP | 1918 | | -23.499 | 20.646 | 1.00 17.10 |
| ATOM | 12854 | | TRP | 1918 | | -26.655 | 18.882 | 1.00 18.69 |
| ATOM | 12855 | NE1 | | 1918 | | -26.300 | 18.691 | 1.00 17.49 |
| ATOM | 12856 | CZ2 | TRP | 1918 | 29.554 | -24.345 | 19.412 | 1.00 14.08 |
| MOTA | 12857 | CZ3 | TRP | 1918 | 30.802 | -22.739 | 20.738 | 1.00 17.47 |
| MOTA | 12858 | CH2 | TRP | 1918 | 29.607 | -23.170 | 20.121 | 1.00 17.12 |
| ATOM | 12859 | C | TRP | 1918 | 33.878 | -26.130 | 22.439 | 1.00 15.03 |
| MOTA | 12860 | 0 | TRP | 1918 | 34.044 | -25.078 | 23.051 | 1.00 15.31 |
| MOTA | 12861 | ·N | LEU | 1919 | | -27.013 | 22.778 | 1.00 14.71 |
| MOTA | 12862 | | LEU | | | -26.761 | | 1.00 14.78 |
| ATOM | 12863 | CB | LEU | 1919 | | ÷27.454 | 23.626 | 1.00 15.37 |
| ATOM ATOM | 12864 12865 | CG CD1 | LEU | 1919 1919 | | -26.866 -27.749 | 22.519 22.330 | 1.00 17.11 1.00 18.09 |
| ATOM | 12866 | | LEU | 1919 | | -27.749 | 22.330 | 1.00 16.88 |
| ATOM | 12867 | C | LEU | 1919 | | -27.206 | 25.259 | 1.00 14.85 |
| ATOM | 12868 | ō | LEU | 1919 | | -26.926 | 26.270 | 1.00 12.57 |
| ATOM | 12869 | N | VAL | 1920 | | -27.893 | 25.298 | 1.00 15.61 |
| ATOM | 12870 | CA | VAL | 1920 | | -28.386 | 26.569 | 1.00 15.42 |
| MOTA | 12871 | CB | VAL | 1920 | | -29.008 | 26.379 | 1.00 16.95 |
| MOTA | 12872 | | VAL | 1920 | 36.302 | -29.125 | 27.717 | 1.00 16.07 |
| MOTA | 12873 | CG2 | VAL | 1920 | 35.425 | -30.389 | 25.764 | 1.00 15.13 |
| MOTA | 12874 | С | VAL | 1920 | | -27.366 | 27.707 | 1.00 16.07 |
| MOTA | 12875 | 0 | VAL | 1920 | , | -27.662 | 28.808 | 1.00 15.60 |
| MOTA | 12876 | N | GLU | 1921 | | -26.172 | 27.448 | 1.00 15.79 |
| MOTA | 12877 | CA | GLU | 1921 | | -25.141 | 28.483 | 1.00 16.09 |
| ATOM | 12878 | CB | GLU | 1921 | | -23.888 | 27.949 | 1.00 18.74 |
| ATOM | 12879 | CG | GLU | 1921 | | -22.701 | 28.889 | 1.00 24.44 |
| ATOM | 12880 | CD OE1 | GLU | 1921 | | -21.543 | 28.394 27.224 | 1.00 27.12 1.00 28.89 |
| ATOM | 12881 | | GLU | 1921 | | -21.136 -21.045 | 27.224 | 1.00 28.89 |
| ATOM ATOM | 12882 12883 | C C | GLU GLU | 1921 1921 | | -21.045 | 28.935 | 1.00 30.38 |
| ATOM | 12884 | 0 | GLU | 1921 | | -24.760 | 30.128 | 1.00 13.04 |
| ATOM | 12885 | N | THR | 1921 | | -24.623 | 27.971 | 1.00 14.33 |
| ATOM | 12886 | CA | THR | 1922 | | -24.268 | 28.289 | 1.00 15.13 |
| MOTA | 12887 | СВ | THR | 1922 | | -24.074 | 27.017 | 1.00 14.39 |
| | | | | | | | | |

| MOTA | 12888 | OG1 | THR | 1922 | 30.846 | -22.993 | 26.265 | 1.00 14.42 |
|--------|-------|-----|-------|------|--------|---------|--------|------------|
| ATOM | 12889 | CG2 | THR | 1922 | 28.834 | -23.753 | 27.354 | 1.00 13.35 |
| ATOM | 12890 | С | THR | 1922 | | -25.321 | 29.161 | 1.00 13.15 |
| ATOM | 12891 | ō | THR | 1922 | | -24.990 | 30.136 | 1.00 13.84 |
| ATOM | 12892 | N | VAL | 1923 | 30.632 | | 28.815 | 1.00 14.02 |
| ATOM | 12893 | CA | VAL | 1923 | 30.042 | -27.671 | 29.590 | 1.00 13.28 |
| ATOM | 12894 | CB | VAL | 1923 | 30.285 | -29.039 | 28.911 | 1.00 13.90 |
| | | | | 1923 | 29.800 | -30.171 | 29.818 | 1.00 14.64 |
| MOTA | 12895 | CG1 | VAL | | | | | |
| MOTA | 12896 | CG2 | VAL | 1923 | 29.552 | -29.080 | 27.584 | 1.00 14.39 |
| MOTA | 12897 | С | VAL | 1923 | 30.611 | | 31.000 | 1.00 15.48 |
| ATOM | 12898 | 0 | VAL | 1923 | 29.863 | -27.755 | 31.982 | 1.00 12.62 |
| ATOM | 12899 | N | GLN | 1924 | 31.932 | -27.598 | 31.109 | 1.00 15.37 |
| ATOM | 12900 | CA | GLN | 1924 | 32,566 | -27.606 | 32.434 | 1.00 17.23 |
| MOTA | 12901 | CB | GLN | 1924 | 34.087 | -27.396 | 32.310 | 1.00 19.46 |
| ATOM | 12902 | CG | GLN | 1924 | 34.796 | -28.434 | 31.437 | 1.00 23.92 |
| ATOM | 12903 | CD | GLN | 1924 | 36.306 | -28.223 | 31.344 | 1.00 28.58 |
| ATOM | 12904 | OE1 | GLN | 1924 | 36.778 | -27.120 | 31.054 | 1.00 27.54 |
| ATOM | 12905 | NE2 | GLN | 1924 | | -29.293 | 31.575 | 1.00 28.43 |
| ATOM | 12906 | C | GLN | 1924 | | -26.527 | 33.344 | 1.00 16.21 |
| ATOM | 12907 | ō | GLN | 1924 | | -26.811 | 34.470 | 1.00 15.27 |
| ATOM | 12908 | N | MET | 1925 | | -25.299 | 32.843 | 1.00 15.24 |
| | 12909 | | | 1925 | | -24.188 | 33.624 | 1.00 13.24 |
| MOTA | | CA | MET | 1925 | | | | 1.00 14.73 |
| MOTA | 12910 | CB | MET | | | -22.875 | 32.921 | |
| MOTA | 12911 | CG | MET | 1925 | | -22.574 | 32.914 | 1.00 17.57 |
| MOTA | 12912 | SD | MET | 1925 | | -21.081 | 31.980 | 1.00 19.95 |
| ATOM | 12913 | CE | MET | 1925 | | -19.842 | 33.296 | 1.00 22.55 |
| ATOM | 12914 | С | MET | 1925 | | -24.267 | 33.944 | 1.00 15.19 |
| MOTA | 12915 | 0 | MET | 1925 | 29.452 | -23.902 | 35.044 | 1.00 12.00 |
| ATOM | 12916 | N | LEU | 1926 | 29.070 | -24.735 | 32.995 | 1.00 13.48 |
| MOTA | 12917 | CA | LEU | 1926 | 27.638 | -24.868 | 33.240 | 1.00 14.38 |
| ATOM | 12918 | CB | LEU | 1926 | 26.934 | -25.398 | 31.989 | 1.00 12.37 |
| ATOM | 12919 | CG | LEU | 1926 | 26.531 | -24.365 | 30.944 | 1.00 10.67 |
| ATOM | 12920 | | LEU | 1926 | | -25.077 | 29.631 | 1.00 10.46 |
| ATOM | 12921 | | LEU | 1926 | 25.320 | | 31.450 | 1.00 11.83 |
| ATOM | 12922 | C | LEU . | | | -25.827 | 34.391 | 1.00 15.78 |
| | | 0 | | 1926 | | -25.542 | 35.298 | 1.00 14.90 |
| ATOM | 12923 | | LEU | | | | | |
| MOTA | 12924 | N | THR | 1927 | 28.061 | | 34.348 | |
| MOTA | 12925 | CA | THR | 1927 | 27.891 | -27.988 | 35.385 | 1.00 19.33 |
| ATOM | 12926 | CB | THR | 1927 | 28.736 | -29.236 | 35.074 | 1.00 22.11 |
| MOTA | 12927 | OG1 | | 1927 | | -29.852 | 33.873 | 1.00 23.96 |
| MOTA | 12928 | CG2 | THR | 1927 | 28.653 | -30.240 | 36.219 | 1.00 26.37 |
| ATOM | 12929 | С | THR | 1927 | 28.222 | -27.472 | 36.780 | 1.00 20.67 |
| ATOM | 12930 | 0 | THR | 1927 | 27.482 | -27.738 | 37.731 | 1.00 19.83 |
| ATOM | 12931 | N | GLU | 1928 | 29.325 | -26.741 | 36.926 | 1.00 19.57 |
| MOTA | 12932 | CA | GLU | 1928 | 29.639 | -26.217 | 38.254 | 1.00 20.59 |
| ATOM · | 12933 | CB | GLU | 1928 | 31.087 | -25.716 | 38.340 | 1.00 23.01 |
| ATOM | 12934 | CG | GLU | 1928 | 31.562 | -24.901 | 37.176 | 1.00 24.98 |
| ATOM | 12935 | CD | GLU | 1928 | 32.983 | -24.379 | 37.372 | 1.00 25.34 |
| ATOM | 12936 | | GLU | 1928 | 33.819 | -25.097 | 37.963 | 1.00 28.59 |
| ATOM | 12937 | OE2 | GLU | 1928 | 33.271 | -23.258 | 36.920 | 1.00 24.69 |
| | | | | 1928 | 28.648 | -25.121 | 38.649 | 1.00 19.64 |
| ATOM | 12938 | C | GLU | | | | | |
| ATOM | 12939 | 0 | GLU | 1928 | | -24.801 | 39.830 | 1.00 20.05 |
| ATOM | 12940 | N | ARG | 1929 | | -24.558 | 37.666 | 1.00 16.54 |
| ATOM | 12941 | CA | ARG | 1929 | 26.938 | -23.536 | 37.948 | 1.00 15.92 |
| MOTA | 12942 | CB | ARG | 1929 | 27.001 | | 36.901 | 1.00 15.43 |
| ATOM | 12943 | CG | ARG | 1929 | 28.222 | -21.543 | 37.095 | 1.00 16.86 |
| MOTA | 12944 | CD | ARG | 1929 | 28.530 | -20.685 | 35.884 | 1.00 16.91 |
| MOTA | 12945 | NE | ARG | 1929 | 29.786 | -19.956 | 36.071 | 1.00 15.63 |
| ATOM | 12946 | CZ | ARG | 1929 | 30.972 | -20.533 | 36.258 | 1.00 17.47 |
| ATOM | 12947 | NH1 | ARG | 1929 | 31.080 | -21.855 | 36.284 | 1.00 20.43 |
| ATOM | 12948 | | ARG | 1929 | 32.056 | -19.786 | 36.418 | 1.00 17.19 |
| ATOM | 12949 | С | ARG | 1929 | 25.531 | -24.134 | 38.032 | 1.00 16.03 |
| ATOM | 12950 | ō | ARG | 1929 | 24.528 | -23.480 | 37.724 | 1.00 15.35 |
| ATOM | 12951 | N | ALA | 1930 | 25.492 | -25.398 | 38.446 | 1.00 15.30 |
| | | | | 1930 | 24.262 | -26.152 | 38.674 | 1.00 13.30 |
| MOTA | 12952 | CA | ALA | | | | | |
| MOTA | 12953 | CB | ALA | 1930 | 23.364 | -25.373 | 39.645 | |
| ATOM | 12954 | С | ALA | 1930 | 23.437 | | 37.473 | 1.00 14.90 |
| ATOM | 12955 | 0 | ALA | 1930 | 22.302 | -27.051 | 37.655 | 1.00 12.87 |
| MOTA | 12956 | N | VAL | 1931 | 23.974 | -26.510 | 36.260 | 1.00 13.13 |
| ATOM | 12957 | CA | VAL | 1931 | 23.217 | -26.948 | 35.100 | 1.00 13.22 |
| MOTA | 12958 | CB | VAL | 1931 | 23.220 | -25.876 | 33.974 | 1.00 14.49 |
| MOTA | 12959 | CG1 | | 1931 | 22.325 | -26.328 | 32.829 | 1.00 11.71 |
| MOTA | 12960 | CG2 | VAL | 1931 | 22.746 | -24.539 | 34.522 | 1.00 14.16 |
| ATOM | 12961 | С | VAL | 1931 | 23.752 | -28.239 | 34.492 | 1.00 13.32 |
| ATOM | 12962 | 0 | VAL | 1931 | 24.905 | -28.296 | 34.046 | 1.00 13.87 |
| ATOM | 12963 | N | PRO | 1932 | | -29.307 | 34.502 | 1.00 13.80 |
| ATOM | 12964 | CD | PRO | 1932 | | -29.508 | 35.290 | 1.00 14.21 |
| | 22703 | | | | , | | | _ |

| ATOM | 12965 | CA | PRO | 1932 | 23.395 | -30.567 | 33.908 | 1.00 13.32 |
|--------|-------|-----|------|------|--------|---------|--------|------------|
| ATOM | 12966 | CB | PRO | 1932 | | -31.596 | 34.437 | 1.00 15.25 |
| | 12967 | CG | PRO | 1932 | | -30.791 | 34.712 | 1.00 20.66 |
| MOTA | | | | | | | | |
| MOTA | 12968 | C | PRO | 1932 | | -30.391 | 32.396 | 1.00 11.97 |
| MOTA | 12969 | 0 | PRO | 1932 | 22.413 | -29.713 | 31.897 | 1.00 12.08 |
| MOTA | 12970 | N | VAL | 1933 | 24.228 | -31.012 | 31.669 | 1.00 11.35 |
| ATOM | 12971 | CA | VAL | 1933 | 24.270 | -30.869 | 30.218 | 1.00 11.25 |
| ATOM | 12972 | СВ | VAL | 1933 | | -30.149 | 29.793 | 1.00 12.56 |
| | | | | | | | | |
| MOTA | 12973 | | VAL | 1933 | | -30.079 | 28.280 | 1.00 10.86 |
| MOTA | 12974 | CG2 | VAL | 1933 | | -28.768 | 30.411 | 1.00 10.60 |
| MOTA | 12975 | C | VAL | 1933 | 24.205 | -32.194 | 29.474 | 1.00 13.16 |
| MOTA | 12976 | 0 | VAL | 1933 | 24.850 | -33.170 | 29.853 | 1.00 12.41 |
| MOTA | 12977 | N | CYS | 1934 | 23 417 | -32.218 | 28.411 | 1.00 11.26 |
| | 12978 | CA | CYS | 1934 | | -33.393 | 27.574 | 1.00 11.02 |
| MOTA | | | | | | | | |
| MOTA | 12979 | CB | CYS | 1934 | | -33.687 | 27.271 | 1.00 11.90 |
| ATOM | 12980 | SG | CYS | 1934 | | -35.022 | 26.038 | 1.00 13.45 |
| ATOM | 12981 | С | CYS | 1934 | 24.031 | -32.993 | 26.301 | 1.00 13.27 |
| ATOM | 12982 | 0 | CYS | 1934 | 23.773 | -31.929 | 25.739 | 1.00 12.86 |
| ATOM | 12983 | N | GLY | 1935 | 24.978 | -33.817 | 25.872 | 1.00 12.09 |
| ATOM | 12984 | CA | GLY | 1935 | | -33.515 | 24.655 | 1.00 10.39 |
| | | | | | | | | |
| MOTA | 12985 | С | GLY | 1935 | | -33.961 | 23.475 | 1.00 11.98 |
| MOTA | 12986 | 0 | GLY | 1935 | 23.843 | -34.627 | 23.654 | 1.00 12.33 |
| MOTA | 12987 | N | HIS | 1936 | 25.305 | -33.601 | 22.272 | 1.00 10.95 |
| MOTA | 12988 | CA | HIS | 1936 | 24.585 | -33.957 | 21.054 | 1.00 13.54 |
| ATOM | 12989 | CB | HIS | 1936 | | -32.945 | 20.813 | 1.00 13.71 |
| | | | | | | -33.285 | 19.669 | 1.00 16.35 |
| MOTA | 12990 | CG | HIS | 1936 | | | | |
| MOTA | 12991 | | HIS | 1936 | 22.722 | -34.088 | 18.593 | 1.00 17.45 |
| MOTA | 12992 | ND1 | HIS | 1936 | 21.297 | -32.719 | 19.522 | 1.00 13.36 |
| ATOM | 12993 | CE1 | HIS | 1936 | 20.745 | -33.155 | 18.406 | 1.00 17.41 |
| MOTA | 12994 | NE2 | | 1936 | 21.589 | -33.986 | 17.821 | 1.00 19.02 |
| | 12995 | C | HIS | 1936 | | -33.974 | 19.889 | 1.00 12.21 |
| ATOM | | | | | | | | |
| ATOM | 12996 | О | HIS | 1936 | | -32.929 | 19.460 | 1.00 12.99 |
| MOTA | 12997 | N | LEU | 1937 | 25.825 | -35.176 | 19.382 | 1.00 13.16 |
| ATOM | 12998 | CA | LEU | 1937 | 26.767 | -35.384 | 18.287 | 1.00 12.94 |
| MOTA | 12999 | CB | LEU | 1937 | 27.994 | -36.157 | 18.797 | 1.00 12.68 |
| ATOM | 13000 | CG | LEU | 1937 | | -35.486 | 19.884 | 1.00 13.53 |
| | | | | | | -36.448 | 20.395 | 1.00 15.18 |
| MOTA | 13001 | CD1 | | 1937 | | | | |
| MOTA | 13002 | CD2 | | 1937 | 29.449 | | 19.334 | 1.00 12.64 |
| MOTA | 13003 | C | LEU | 1937 | 26.141 | -36.137 | 17.126 | 1.00 14.83 |
| ATOM | 13004 | 0 | LEU | 1937 | 25.103 | -36.785 | 17.274 | 1.00 12.98 |
| ATOM | 13005 | N | GLY | 1938 | 26.792 | -36.055 | 15.972 | 1.00 16.63 |
| ATOM | 13006 | CA | GLY | 1938 | | -36.719 | 14.790 | 1.00 22.86 |
| | | | | | | | | |
| MOTA | 13007 | C | GLY | 1938 | | -35.675 | 13.854 | 1.00 27.34 |
| MOTA | 13008 | 0 | GLY | 1938 | | -34.740 | 13.466 | 1.00 27.92 |
| ATOM | 13009 | N | LEU | 1939 | 24.438 | -35.824 | 13.504 | 1.00 30.73 |
| ATOM | 13010 | CA | LEU | 1939 | 23.766 | -34.889 | 12.611 | 1.00 34.21 |
| ATOM | 13011 | CB | LEU | 1939 | | -35.638 | 11.786 | 1.00 35.61 |
| MOTA | 13012 | CG | LEU | 1939 | | -34.928 | 10.615 | 1.00 37.63 |
| | | | | | | | | |
| MOTA | 13013 | CD1 | | 1939 | | -35.969 | 9.702 | 1.00 38.32 |
| MOTA | 13014 | CD2 | LEU | 1939 | 20.973 | -33.955 | 11.127 | 1.00 38.51 |
| ATOM | 13015 | С | LEU | 1939 | 23.116 | -33.768 | 13.420 | 1.00 36.56 |
| ATOM | 13016 | 0 | LEU | 1939 | 22.114 | -33.980 | 14.101 | 1.00 37.71 |
| ATOM | 13017 | N | THR | 1940 | | -32.576 | 13.343 | 1.00 38.68 |
| ATOM | 13018 | CA | THR | 1940 | | -31.417 | 14.070 | 1.00 40.34 |
| | | | | | 24.337 | | | 1.00 40.75 |
| MOTA | 13019 | CB | THR | 1940 | | -30.684 | 14.791 | |
| ATOM | 13020 | OG1 | | 1940 | 25.398 | -30.420 | 13.864 | 1.00 39.49 |
| ATOM | 13021 | CG2 | THR | 1940 | 24.867 | -31.530 | 15.934 | 1.00 41.22 |
| MOTA | 13022 | С | THR | 1940 | 22.490 | -30.447 | 13.124 | 1.00 41.01 |
| ATOM | 13023 | ō | THR | 1940 | | | 12.379 | 1.00 42.38 |
| | 13024 | | | 1941 | | -30.430 | 13.152 | 1.00 42.07 |
| ATOM | | N | PRO | | | | | |
| ATOM | 13025 | CD | PRO | 1941 | | -31.239 | 14.041 | 1.00 43.13 |
| MOTA | 13026 | CA | PRO | 1941 | 20.333 | -29.558 | 12.297 | 1.00 42.02 |
| MOTA | 13027 | CB | PRO | 1941 | 18.903 | -29.997 | 12.615 | 1.00 42.88 |
| ATOM | 13028 | CG | PRO | 1941 | 18.995 | -30.474 | 14.019 | 1.00 44.03 |
| ATOM | 13029 | C | PRO | 1941 | | -28.058 | 12.486 | 1.00 41.54 |
| | | | | 1941 | | -27.265 | 11.611 | 1.00 41.77 |
| MOTA | 13030 | 0 | PRO | | | | | |
| MOTA | 13031 | N | GLN | 1942 | 21.121 | | 13.619 | 1.00 40.66 |
| MOTA | 13032 | CA | GLN | 1942 | | -26.245 | 13.857 | 1.00 40.39 |
| MOTA | 13033 | CB | GLN | 1942 | | -26.012 | 15.307 | 1.00 39.97 |
| MOTA | 13034 | CG | GLN | 1942 | 20.658 | -25.656 | 16.244 | 1.00 38.76 |
| ATOM | 13035 | CD | GLN | 1942 | | -25.620 | 17.701 | 1.00 38.71 |
| | | | | | | -24.999 | 18.053 | 1.00 35.82 |
| ATOM | 13036 | | GLN | 1942 | | | | |
| MOTA | 13037 | NE2 | | 1942 | | -26.284 | 18.559 | 1.00 36.70 |
| MOTA | 13038 | С | GLN | 1942 | | -25.722 | 12.906 | 1.00 40.11 |
| ATOM | 13039 | 0 | GLN | 1942 | 22.541 | -24.519 | 12.660 | 1.00 39.36 |
| ATOM | 13040 | N | SER | 1943 | | -26.637 | 12.372 | 1.00 40.02 |
| ATOM | | CA | SER | 1943 | | -26.281 | 11.443 | 1.00 39.90 |
| 111 OF | 13041 | CA | Acto | 1743 | 44.367 | 20.201 | | |
| | | | | | | | | |

| ATOM | 13042 | СВ | SER | 1943 | 25.637 | -26.959 | 11.862 | 1.00 40.15 |
|--------------|----------------|----------|------------|--------------|--------|--------------------|----------------|--------------------------|
| ATOM | 13043 | OG | SER | 1943 | | -26.629 | 13.195 | 1.00 42.09 |
| ATOM | 13044 | C | SER | 1943 | | -26.703 | 10.017 | 1.00 39.67 |
| MOTA | 13045 | ō | SER | 1943 | | -26.933 | 9.194 | 1.00 38.51 |
| ATOM | 13046 | N | VAL | 1944 | 22.682 | -26.805 | 9.734 | 1.00 40.21 |
| MOTA | 13047 | CA | VAL | 1944 | 22.209 | -27.205 | 8.411 | 1.00 40.13 |
| MOTA | 13048 | CB | VAL | 1944 | 20.660 | -27.155 | 8.335 | 1.00 40.32 |
| MOTA | 13049 | CG1 | VAL | 1944 | 20.160 | -25.763 | 8.698 | 1.00 40.26 |
| ATOM | 13050 | CG2 | VAL | 1944 | 20.196 | -27.547 | 6.936 | 1.00 40.12 |
| ATOM | 13051 | С | VAL | 1944 | 22.794 | -26.352 | 7.284 | 1.00 40.09 |
| ATOM | 13052 | 0 | VAL | 1944 | 23.178 | -26.873 | 6.236 | 1.00 40.03 |
| MOTA | 13053 | N | ASN | 1945 | 22.862 | -25.043 | 7.501 | 1.00 40.77 |
| MOTA | 13054 | CA | ASN | 1945 | 23.397 | -24.128 | 6.498 | 1.00 42.02 |
| MOTA | 13055 | CB | ASN | 1945 | 23.120 | -22.681 | 6.911 | 1.00 39.36 |
| MOTA | 13056 | CG | ASN | 1945 | 21.634 | -22.388 | 7.028 | 1.00 38.68 |
| MOTA | 13057 | OD1 | ASN | 1945 | | -22.428 | 6.035 | 1.00 33.53 |
| MOTA | 13058 | | ASN | 1945 | | -22.102 | 8.244 | 1.00 34.93 |
| MOTA | 13059 | С | ASN | 1945 | | -24.336 | 6.292 | 1.00 43.74 |
| ATOM | 13060 | 0 | ASN | 1945 | | -24.102 | 5.200 | 1.00 43.69 |
| ATOM | 13061 | N | ILE | 1946 | | -24.774 | 7.344 | 1.00 46.06 |
| MOTA | 13062 | CA | ILE | 1946 | | -25.024 | 7.275 | 1.00 48.85 |
| MOTA | 13063 | CB | ILE | 1946 | | -25.387 | 8.664 | 1.00 48.08 |
| MOTA | 13064 | CG2 | | 1946 | | -25.828 | 8.527 | 1.00 48.67 |
| MOTA | | CG1 | ILE | 1946 | | -24.188 | 9.609 | 1.00 47.10 |
| ATOM | 13066 | | ILE | 1946 | | -22.994 | 9.203 | 1.00 45.47 |
| ATOM | 13067 | C | ILE | 1946 | | -26.176 | 6.316 | 1.00 51.55 1.00 51.88 |
| ATOM | 13068 | 0 | ILE | 1946 | | -26.001 | 5.287 | |
| MOTA | | . N | | 1947 | | -27.354 -28.551 | 6,666 5.855 | 1.00 54.57 1.00 57.12 |
| MOTA | 13070 | CA | PHE | 1947 1947 | | -28.551 | 6.605 | 1.00 57.12 |
| MOTA MOTA | 13071 13072 | CB CG | PHE PHE | 1947 | | -30.023 | 7.924 | 1.00 59.02 |
| ATOM | 13072 | | PHE | 1947 | | -30.544 | 7.969 | 1.00 62.43 |
| ATOM | 13073 | | PHE | 1947 | | -29.726 | 9.121 | 1.00 61.93 |
| ATOM | 13074 | | PHE | 1947 | | -30.767 | 9.189 | 1.00 62.77 |
| MOTA | 13075 | | PHE | 1947 | | -29.945 | 10.345 | 1.00 62.58 |
| MOTA | 13077 | CZ | PHE | 1947 | | -30.467 | 10.379 | 1.00 62.90 |
| ATOM | 13078 | C | PHE | 1947 | | -28.407 | 4.514 | 1.00 58.08 |
| ATOM | 13079 | Ô | PHE | 1947 | | -28.505 | 3.455 | 1.00 59.24 |
| ATOM | 13080 | N | GLY | 1948 | | -28.169 | 4.566 | 1.00 58.06 |
| ATOM | 13081 | CA | GLY | 1948 | | -28.015 | 3.349 | 1.00 58.62 |
| ATOM | 13082 | C | GLY | 1948 | | -28.761 | 3.410 | 1.00 59.00 |
| ATOM | 13083 | 0 | GLY | 1948 | | -28.740 | 2.458 | 1.00 58.82 |
| MOTA | 13084 | N | GLY | 1949 | 22.613 | -29.420 | 4.537 | 1.00 59.35 |
| MOTA | 13085 | CA | GLY | 1949 | 21.381 | -30.168 | 4.701 | 1.00 60.55 |
| ATOM | 13086 | С | GLY | 1949 | 21.459 | -31.129 | 5.870 | 1.00 61.51 |
| ATOM | 13087 | 0 | GLY | 1949 | 22.026 | -30.801 | 6.914 | 1.00 61.37 |
| MOTA | 13088 | N | TYR | 1950 | 20.889 | -32.319 | 5.695 | 1.00 62.15 |
| MOTA | 13089 | CA | TYR | 1950 | 20.898 | -33.337 | 6.745 | 1.00 62.76 |
| MOTA | 13090 | CB | TYR | 1950 | 19.524 | -33.419 | 7.420 | 1.00 63.27 |
| MOTA | 13091 | CG | TYR | 1950 | 18.892 | -32.075 | 7.706 | 1.00 63.93 |
| MOTA | 13092 | CD1 | TYR | 1950 | 18.228 | -31.368 | 6.702 | 1.00 64.37 |
| MOTA | 13093 | | TYR | 1950 | | -30.124 | 6.955 | 1.00 64.90 |
| ATOM | 13094 | | TYR | 1950 | | -31.502 | 8.975 | 1.00 64.29 |
| MOTA | 13095 | CE2 | TYR | 1950 | | -30.258 | 9.239 | 1.00 64.47 |
| ATOM | 13096 | CZ | TYR | 1950 | | -29.576 | 8.225 | 1.00 65.14 |
| ATOM | 13097 | OH | TYR | 1950 | | -28.347 | 8.477 | 1.00 65.21 |
| MOTA | 13098 | C | TYR | 1950 | | -34.703 | 6.163 | 1.00 62.54 |
| ATOM | 13099 | 0 | TYR | 1950 | | -35.272 | 5.371 | 1.00 62.37 |
| ATOM | 13100 | N | LYS | 1951 | | -35.223 -36.517 | 6.564 | 1.00 62.40 |
| ATOM | 13101 | CA | LYS | 1951 | | -36.517 | 6.081 4.919 | 1.00 62.04 1.00 62.86 |
| MOTA MOTA | 13102 13103 | CB CG | LYS LYS | 1951 1951 | | -36.315 | 3.721 | 1.00 62.86 |
| | | | | | | -35.241 | 2.688 | 1.00 65.92 |
| ATOM ATOM | 13104 13105 | CD | LYS LYS | 1951 1951 | | -34.471 | 1.532 | 1.00 65.32 |
| ATOM | 13105 | NZ | LYS | 1951 | | -33.991 | 0.560 | 1.00 67.31 |
| ATOM | 13107 | C | LYS | 1951 | | -37.316 | 7.190 | 1.00 60.75 |
| ATOM | 13107 | 0 | LYS | 1951 | | -36.755 | 8.195 | 1.00 60.75 |
| ATOM | 13100 | N | VAL | 1952 | | -38.630 | 6.999 | 1.00 58.89 |
| MOTA | 13110 | CA | VAL | 1952 | | -39.511 | 7.979 | 1.00 57.24 |
| ATOM | 13111 | CB | VAL | 1952 | | -40.975 | 7.491 | 1.00 57.00 |
| ATOM | 13112 | | VAL | 1952 | | -41.875 | 8.545 | 1.00 57.09 |
| ATOM | 13113 | CG2 | | 1952 | | -41.422 | 7.184 | 1.00 56.86 |
| MOTA | 13114 | C | VAL | 1952 | | -39.079 | 8.243 | 1.00 56.27 |
| MOTA | 13115 | ō | VAL | 1952 | | -38.917 | 7.313 | 1.00 55.83 |
| MOTA | 13116 | N | GLN | 1953 | | -38.898 | 9.517 | 1.00 54.84 |
| MOTA | 13117 | CA | GLN | 1953 | 27.395 | -38.479 | 9.907 | 1.00 53.67 |
| MOTA | 13118 | СВ | GLN | 1953 | 27.303 | -37.270 | 10.841 | 1.00 53.92 |
| | | | | | | | | |

| ATOM | 13119 | CG | GLN | 1953 | 28.623 -36.560 | 11.083 | 1.00 55.91 |
|------|-------|-----|-----|------|----------------|-----------------|--------------------------|
| ATOM | 13120 | CD | GLN | 1953 | 29.188 -35.934 | 9.820 | 1.00 56.76 |
| ATOM | 13121 | OE1 | GLN | 1953 | 28.532 -35.114 | 9.174 | 1.00 55.89 |
| ATOM | 13122 | NE2 | GLN | 1953 | 30.413 -36.318 | 9.463 | 1.00 56.77 |
| ATOM | 13123 | С | GLN | 1953 | 28.137 -39.623 | 10.600 | 1.00 52.67 |
| ATOM | 13124 | Ō | GLN | 1953 | 27.517 -40.550 | 11.116 | 1.00 52.18 |
| ATOM | 13125 | N | GLY | 1954 | 29.466 -39.558 | 10.598 | 1.00 51.97 |
| ATOM | 13126 | CA | GLY | 1954 | 30.256 -40.598 | 11.236 | 1.00 51.94 |
| ATOM | 13127 | C | GLY | 1954 | 30.855 -41.601 | 10.266 | 1.00 51.75 |
| ATOM | 13128 | ō | GLY | 1954 | 31.612 -42.488 | 10.664 | 1.00 51.15 |
| ATOM | 13129 | N | ARG | 1955 | 30.514 -41.462 | 8.990 | 1.00 51.95 |
| ATOM | 13130 | CA | ARG | 1955 | 31.018 -42.353 | 7.953 | 1.00 52.89 |
| ATOM | 13131 | CB | ARG | 1955 | 30.331 -42.042 | 6.619 | 1.00 54.06 |
| ATOM | 13132 | CG | ARG | 1955 | 28.840 -42.353 | 6.588 | 1.00 56.32 |
| ATOM | 13133 | CD | ARG | 1955 | 28.588 -43.852 | 6.597 | 1.00 58.03 |
| ATOM | 13134 | NE | ARG | 1955 | 27.164 -44.184 | 6.599 | 1.00 59.33 |
| ATOM | 13135 | CZ | ARG | 1955 | 26.313 -43.872 | 5.625 | 1.00 59.73 |
| ATOM | 13136 | NH1 | | 1955 | 26.735 -43.212 | 4.554 | 1.00 59.72 |
| ATOM | 13137 | NH2 | ARG | 1955 | 25.036 -44.223 | 5.720 | 1.00 60.10 |
| MOTA | 13138 | C | ARG | 1955 | 32.529 -42.205 | 7.797 | 1.00 52.91 |
| ATOM | 13139 | Ö | ARG | 1955 | 33.034 -41.102 | 7.582 | 1.00 52.93 |
| ATOM | 13140 | N | GLY | 1956 | 33.245 -43.320 | 7.909 | 1.00 52.81 |
| ATOM | 13141 | CA | GLY | 1956 | 34.692 -43.290 | 7.771 | 1.00 52.45 |
| ATOM | 13142 | C | GLY | 1956 | 35.420 -43.286 | 9.101 | 1.00 51.95 |
| ATOM | 13143 | ō | GLY | 1956 | 34.882 -42.834 | 10.110 | 1.00 52.28 |
| MOTA | 13144 | N | ASP | 1957 | 36.650 -43.787 | 9.101 | 1.00 51.06 |
| ATOM | 13145 | CA | ASP | 1957 | 37.450 -43.841 | 10.319 | 1.00 50.18 |
| | 13145 | CB | ASP | 1957 | 38.777 -44.553 | 10.050 | 1.00 50.18 |
| MOTA | | | | | 38.584 -45.974 | 9.572 | 1.00 55.34 |
| MOTA | 13147 | CG | ASP | 1957 | | | |
| MOTA | 13148 | | ASP | 1957 | 37.909 -46.752 | 10.283 8.489 | 1.00 56.35 1.00 57.00 |
| MOTA | 13149 | OD2 | | 1957 | 39.109 -46.315 | | |
| MOTA | 13150 | C | ASP | 1957 | 37.727 -42.446 | 10.867 | 1.00 47.95 |
| MOTA | 13151 | 0 | ASP | 1957 | 37.620 -42.209 | 12.069 | 1.00 47.47 |
| ATOM | 13152 | N | GLU | 1958 | 38.087 -41.529 | 9.977 | 1.00 45.13 |
| MOTA | 13153 | CA | GLU | 1958 | 38.387 -40.160 | 10.368 | 1.00 43.01 |
| ATOM | 13154 | CB | GLU | 1958 | 38.677 -39.318 | 9.127 | 1.00 45.74 |
| MOTA | 13155 | CG | GLU | 1958 | 39.190 -37.924 | 9.429 | 1.00 48.92 |
| MOTA | 13156 | CD | GLU | 1958 | 39.353 -37.092 | 8.174 | 1.00 51.94 |
| MOTA | 13157 | OE1 | | 1958 | 39.989 -37.585 | 7.215 | 1.00 52.78 |
| MOTA | 13158 | OE2 | GLU | 1958 | 38.850 -35.947 | 8.148 | 1.00 53.38 |
| MOTA | 13159 | С | GLU | 1958 | 37.231 -39.540 | 11.146 | 1.00 40.27 |
| MOTA | 13160 | 0 | GLU | 1958 | 37.380 -39.175 | 12.313 | 1.00 37.28 |
| MOTA | 13161 | N | ALA | 1959 | 36.079 -39.424 | 10.493 | 1.00 36.37 |
| MOTA | 13162 | CA | ALA | 1959 | 34.900 -38.846 | 11.129 | 1.00 34.01 |
| MOTA | 13163 | CB | ALA | 1959 | 33.754 -38.760 | 10.130 | 1.00 33.11 |
| MOTA | 13164 | Ç | ALA | 1959 | 34.484 -39.683 | 12.333 | 1.00 31.93 |
| MOTA | 13165 | 0 | ALA | 1959 | 34.046 -39.149 | 13.353 | 1.00 31.65 |
| MOTA | 13166 | N | GLY | 1960 | 34.625 -40.997 | 12.203 | 1.00 30.55 |
| MOTA | 13167 | CA | GLY | 1960 | 34.262 -41.895 | 13.283 | 1.00 29.48 |
| ATOM | 13168 | C | GLY | 1960 | 35.089 -41.676 | 14.535 | 1.00 28.48 |
| MOTA | 13169 | 0 | GLY | 1960 | 34.553 -41.644 | 15.644 | 1.00 27.01 |
| MOTA | 13170 | N | ASP | 1961 | 36.397 -41.520 | 14.365 | 1.00 27.04 |
| MOTA | 13171 | CA | ASP | 1961 | 37.284 -41.310 | 15.502 | 1.00 27.15 |
| MOTA | 13172 | CB | ASP | 1961 | 38.752 -41.439 | 15.076 | 1.00 29.17 |
| MOTA | 13173 | CG | ASP | 1961 | 39.120 -42.849 | 14.653 | 1.00 31.98 |
| MOTA | 13174 | OD1 | ASP | 1961 | 38.398 -43.797 | 15.040 | 1.00 30.19 |
| MOTA | 13175 | OD2 | ASP | 1961 | 40.143 -43.009 | 13.944 | 1.00 33.17 |
| MOTA | 13176 | C | ASP | 1961 | 37.053 -39.947 | 16.135 | 1.00.25.99 |
| MOTA | 13177 | 0 | ASP | 1961 | 37.114 -39.803 | 17.358 | 1.00 25.23 |
| MOTA | 13178 | N | GLN | 1962 | 36.791 -38.945 | 15.301 | 1.00 24.65 |
| MOTA | 13179 | CA | GLN | 1962 | 36.549 -37.598 | 15.803 | 1.00 24.43 |
| MOTA | 13180 | CB | GLN | 1962 | 36.404 -36.613 | 14.644 | 1.00 25.79 |
| MOTA | 13181 | CG | GLN | 1962 | 36.228 -35.174 | 15.095 | 1.00 28.89 |
| MOTA | 13182 | CD | GLN | 1962 | 37.400 -34.677 | 15.912 | 1.00 31.20 |
| MOTA | 13183 | OE1 | GLN | 1962 | 38.524 -34.600 | 15.419 | 1.00 31.16 |
| ATOM | 13184 | NE2 | GLN | 1962 | 37.144 -34.339 | 17.172 | 1.00 32.91 |
| ATOM | 13185 | С | GLN | 1962 | 35.295 -37.556 | 16.678 | 1.00 22.32 |
| MOTA | 13186 | ō | GLN | 1962 | 35.267 -36.860 | 17.691 | 1.00 20.87 |
| ATOM | 13187 | N | LEU | 1963 | 34.258 -38.294 | 16.285 | 1.00 21.33 |
| MOTA | 13188 | CA | LEU | 1963 | 33.032 -38.323 | 17.068 | 1.00 21.71 |
| MOTA | 13189 | CB | LEU | 1963 | 31.900 -39.012 | 16.293 | 1.00 22.46 |
| MOTA | 13190 | CG | LEU | 1963 | 31.338 -38.237 | 15.092 | 1.00 28.54 |
| ATOM | 13191 | | LEU | 1963 | 30.208 -39.027 | 14.450 | 1.00 28.46 |
| ATOM | 13192 | | LEU | 1963 | 30.822 -36.868 | 15.550 | 1.00 27.56 |
| ATOM | 13193 | C | LEU | 1963 | 33.274 -39.044 | 18.392 | 1.00 20.51 |
| ATOM | 13194 | o | LEU | 1963 | 32.745 -38.641 | . 19.425 | 1.00 18.17 |
| ATOM | 13195 | N | LEU | 1964 | 34.074 -40.109 | 18.359 | 1.00 19.90 |
| | | | | | | | |

| MOTA | 13196 | CA | LEU | 1964 | 34.387 | -40.860 | 19.573 | 1.00 | 18.82 |
|--------------|----------------|-----------|-------|--------------|--------|--------------------|------------------|------|----------------|
| ATOM | 13197 | СВ | LEU | 1964 | | -42.060 | 19.258 | 1.00 | 19.20 |
| ATOM | 13198 | CG | LEU | 1964 | | -43.326 | 20.114 | 1.00 | 22.73 |
| ATOM | 13199 | CD1 | LEU | 1964 | | -44.170 | 19.984 | 1.00 | 21.26 |
| ATOM | 13200 | CD2 | LEU | 1964 | 34.908 | -42.985 | 21.568 | 1.00 | 21.92 |
| MOTA | 13201 | С | LEU | 1964 | 35.125 | -39.916 | 20.513 | 1.00 | 18.01 |
| ATOM | 13202 | 0 | LEU | 1964 | 34.827 | -39.843 | 21.704 | 1.00 | 16.75 |
| ATOM | 13203 | N | SER | 1965 | 36.097 | -39.197 | 19.958 | 1.00 | 19.21 |
| ATOM | 13204 | CA | SER | 1965 | 36.891 | -38.251 | 20.726 | 1.00 | 18.88 |
| MOTA | 13205 | СВ | SER | 1965 | 37.939 | -37.586 | 19.834 | 1.00 | 19.39 |
| ATOM | 13206 | OG | SER | 1965 | 38.736 | -36.691 | 20.592 | 1.00 | 21.10 |
| MOTA | 13207 | С | SER | 1965 | 36.017 | -37.179 | 21.354 | 1.00 | 17.02 |
| MOTA | 13208 | 0 | SER | 1965 | 36.122 | -36.915 | 22.550 | 1.00 | 15.35 |
| ATOM | 13209 | N | ASP | 1966 | 35.156 | -36.558 | 20.549 | 1.00 | 16.60 |
| MOTA | 13210 | CA | ASP | 1966 | 34.278 | -35.509 | 21.071 | 1.00 | 17.92 |
| ATOM | 13211 | CB | ASP | 1966 | 33.404 | -34.910 | 19.964 | 1.00 | 18.63 |
| MOTA | 13212 | CG | ASP | 1966 | 34.197 | -34.078 | 18.974 | 1.00 | 19.16 |
| MOTA | 13213 | OD1 | ASP | 1966 | 35.254 | -33.536 | 19.352 | 1.00 | 24.28 |
| ATOM | 13214 | OD2 | ASP | 1966 | 33.745 | -33.954 | 17.819 | 1.00 | 20.44 |
| ATOM | 13215 | С | ASP | 1966 | 33.378 | -36.061 | 22.170 | 1.00 | 15.95 |
| ATOM | 13216 | 0 | ASP | 1966 | 33.162 | -35.409 | 23.194 | 1.00 | 15.58 |
| MOTA | 13217 | N | ALA | 1967 | 32.852 | -37.263 | 21.955 | 1.00 | 15.46 |
| MOTA | 13218 | CA | ALA | 1967 | 31.980 | -37.889 | 22.946 | 1.00 | 13.99 |
| MOTA | 13219 | CB | ALA | 1967 | 31.536 | -39.264 | 22.454 | 1.00 | 13.81 |
| MOTA | 13220 | С | ALA | 1967 | 32.703 | -38.012 | 24.280 | 1.00 | 14.10 |
| ATOM | 13221 | 0 | ALA | 1967 | 32.157 | -37.674 | 25.333 | 1.00 | 14.44 |
| ATOM | 13222 | N | LEU | 1968 | 33.944 | -38.490 | 24.240 | 1.00 | 13.09 |
| MOTA | 13223 | CA | LEU | 1968 | 34.724 | -38.650 | 25.463 | 1.00 | 13.85 |
| MOTA | 13224 | CB | LEU | 1968 | 36.010 | -39.434 | 25.164 | 1.00 | 14.52 |
| MOTA | 13225 | CG | LEU | 1968 | | -40.946 | 24.954 | 1.00 | |
| MOTA | 13226 | CD1 | LEU | 1968 | | -41.547 | 24.234 | 1.00 | 16.18 |
| MOTA. | 13227 | CD2 | LEU | 1968 | | -41.618 | 26.306 | 1.00 | |
| MOTA | 13228 | С | ĻEU | 1968 | 35.062 | -37.293 | 26.088 | 1.00 | 13.86 |
| ATOM | 13229 | 0 | LEU | 1968 | | -37.157 | 27.309 | 1.00 | 14.68 |
| MOTA | 13230 | N | ALA | 1969 | | -36.290 | 25.257 | 1.00 | |
| MOTA | 13231 | CA | ALA | 1969 | | -34.957 | 25.769 | 1.00 | |
| ATOM | 13232 | CB | ALA | 1969 | | -34.057 | 24.634 | 1.00 | 14.15 |
| MOTA | 13233 | С | ALA | 1969 | | -34.325 | 26.462 | 1.00 | 13.52 |
| MOTA | 13234 | 0 | ALA | 1969 | | -33.634 | 27.476 | 1.00 | 12.39 |
| MOTA | 13235 | N | LEU | 1970 | 33.283 | -34.552 | 25.909 | 1.00 | 15.34 |
| MOTA | 13236 | CA | LEU | 1970 | | -34.005 | 26.502 | 1.00 | |
| MOTA | 13237 | CB | LEU | 1970 | | -34.220 | 25.563 | 1.00 | |
| MOTA | 13238 | CG | LEU | 1970 | | -33.394 | 24.272 | 1.00 | 16.66 |
| ATOM | 13239 | | LEU | 1970 | | -33.811 | 23.329. | 1.00 | 17.51 |
| ATOM | 13240 | | LEU | 1970 | | -31.913 | 24.610 27.848 | 1.00 | 16.43 |
| ATOM | 13241 | C | LEU | 1970 | | -34.661 | | 1.00 | 13.96 12.41 |
| ATOM | 13242 | 0 | LEU | 1970 | | -33.982 -35.980 | 28.824 27.907 | 1.00 | |
| MOTA | 13243 | N | GLU | 1971 | | -36.705 | 29.162 | 1.00 | |
| MOTA | 13244 13245 | CA _ | GLU | 1971 1971 | 31.767 | -38.224 | 28.945 | 1.00 | 16.29 |
| ATOM | 13245 | CG | GLU | 1971 | | -39.074 | 30.226 | 1.00 | 15.90 |
| ATOM | 13246 | | GLU | 1971 | | -40.557 | 29.981 | | 15.83 |
| MOTA MOTA | 13247 | CD OF1 | GLU | 1971 | | -40.888 | 29.415 | | 18.88 |
| ATOM | 13249 | | GLU | 1971 | | -41.392 | 30.358 | 1.00 | 19.45 |
| ATOM | 13250 | C | GLU | 1971 | | -36.207 | 30.195 | 1.00 | 15.16 |
| ATOM | 13251 | ō | GLU | 1971 | 32.465 | -35.965 | 31.353 | 1.00 | 13.13 |
| ATOM | 13252 | N | ALA | 1972 | | -36.039 | 29.774 | 1.00 | 14.67 |
| MOTA | 13253 | CA | ALA | 1972 | | -35.589 | 30.695 | 1.00 | 15.71 |
| ATOM | 13254 | CB | ALA | 1972 | | -35.643 | 30.015 | 1.00 | 15.78 |
| MOTA | 13255 | c | ALA | 1972 | | -34.181 | 31.192 | 1.00 | 15.67 |
| ATOM | 13256 | ō | ALA | 1972 | | -33.832 | 32.323 | 1.00 | 17.06 |
| ATOM | 13257 | N | ALA | 1973 | | -33.377 | 30.342 | 1.00 | 16.83 |
| ATOM | 13258 | CA | ALA | 1973 | | -31.993 | 30.673 | 1.00 | 16.03 |
| ATOM | 13259 | СВ | ALA | 1973 | | -31.243 | 29.399 | 1.00 | 17.16 |
| MOTA | 13260 | С | ALA | 1973 | 32.690 | -31.924 | 31.694 | 1.00 | 16.25 |
| ATOM | 13261 | 0 | ALA | 1973 | | -30.900 | 32.354 | 1.00 | 16.68 |
| MOTA | 13262 | N | GLY " | 1974 | | -33.013 | | 1.00 | 15.27 |
| MOTA | 13263 | ĊA | GLY | 1974 | | -33.037 | 32.790 | 1.00 | 15.24 |
| ATOM | 13264 | C | GLY | 1974 | 29.473 | -33.342 | 32.251 | 1.00 | 13.22 |
| ATOM | 13265 | 0 | GLY | 1974 | 28.498 | -33.327 | 33.008 | 1.00 | 13.69 |
| MOTA | 13266 | N | ALA | 1975 | 29.357 | -33.606 | 30.954 | 1.00 | 13.87 |
| MOTA | 13267 | CA | ALA | 1975 | 28.038 | -33.927 | 30.396 | 1.00 | 12.92 |
| ATOM | 13268 | CB | ALA | 1975 | | -34.066 | 28.888 | 1.00 | 12.07 |
| MOTA | 13269 | C | ALA | 1975 | | -35.243 | 31.031 | 1.00 | 12.54 |
| MOTA | 13270 | 0 | ALA | 1975 | | -36.188 | 31.104 | 1.00 | 11.18 |
| ATOM | 13271 | N | GLN | 1976 | | -35.304 | 31.492 | 1.00 | 11.89 |
| MOTA | 13272 | CA | GLN | 1976 | 25.803 | -36.514 | 32.132 | 1.00 | 11.40 |

| ATOM | 13273 | ĊВ | GLN | 1976 | 25.009 | -36.150 | 33.387 | 1.00 | 12.41 |
|------|--------|-----|-----|---------------|----------|---------|--------|------|-------|
| АТОМ | 13274 | CG | GLN | 1976 | 25.890 | | 34.561 | 1.00 | 15.82 |
| | 13275 | CD | GLN | 1976 | | -35.135 | 35.720 | 1.00 | 16.62 |
| MOTA | | | | | | | | | |
| ATOM | 13276 | OE1 | | 1976 | 24.747 | | 36.671 | | 21.24 |
| ATOM | 13277 | NE2 | GLN | 1976 | 24.784 | -33.847 | 35.641 | 1.00 | 14.90 |
| ATOM | 13278 | С | GLN | 1976 | 24.931 | -37.348 | 31.196 | 1.00 | 11.43 |
| MOTA | 13279 | 0 | GLN | 1976 | 24.407 | -38 397 | 31.581 | 1.00 | 11.61 |
| | | | LEU | 1977 | | -36.862 | 29.970 | 1.00 | 10.84 |
| MOTA | 13280 | N | | | | | | | |
| MOTA | 13281 | CA | LEU | 1977 | 23.986 | | 28.957 | 1.00 | 12.72 |
| MOTA | 13282 | CB | LEU | 1977 | 22.510 | -37.145 | 29.089 | 1.00 | 15.93 |
| ATOM | 13283 | CG | LEU | 1977 | 21.602 | -38.134 | 29.806 | 1.00 | 21.02 |
| ATOM | 13284 | CD1 | LEU | 1977 | 20.255 | -37.461 | 30.072 | 1.00 | 21.00 |
| ATOM | 13285 | CD2 | | 1977 | | -39.379 | 28.955 | | 23.10 |
| | | | | | | | | | |
| ATOM | 13286 | С | LEU | 1977 | | -37.130 | 27.588 | 1.00 | 11.33 |
| MOTA | 13287 | 0 | LEU | 1977 | | -36.050 | 27.414 | 1.00 | 12.24 |
| MOTA | 13288 | N | LEU | 1978 | 24.253 | -38.004 | 26.614 | 1.00 | 11.93 |
| ATOM | 13289 | CA | LEU | 1 9 78 | 24.673 | -37.739 | 25.247 | 1.00 | 12.10 |
| ATOM | 13290 | CB | LEU | 1978 | | -38.341 | 25.001 | 1.00 | 13.29 |
| | 13291 | CG | | 1978 | | -38.431 | 23.533 | 1.00 | 16.13 |
| ATOM | | | LEU | | | | | | |
| MOTA | 13292 | CD1 | | 1978 | | -37.031 | 22.943 | | 16.64 |
| ATOM | 13293 | CD2 | LEU | 1978 | 27.819 | -39.159 | 23.422 | 1.00 | 12.84 |
| MOTA | 13294 | С | LEU | 1978 | 23.688 | -38.311 | 24.238 | 1.00 | 12.27 |
| ATOM | 13295 | 0 | LEU | 1978 | 23.223 | -39.445 | 24.374 | 1.00 | 13.09 |
| | 13296 | N | VAL | 1979 | | -37.503 | 23.239 | 1.00 | 11.61 |
| ATOM | | | | | | | | | |
| MOTA | 13297 | CA | VAL | 1979 | | -37.911 | 22.159 | | 10.55 |
| MOTA | 13298 | CB | VAL | 1979 | 21.370 | -36.815 | 21.854 | 1.00 | 10.14 |
| MOTA | 13299 | CG1 | VAL | 1979 | 20.708 | -37.068 | 20.492 | 1.00 | 10.01 |
| ATOM | 13300 | CG2 | VAL | 1979 | 20.321 | -36.812 | 22.935 | 1.00 | 9.21 |
| ATOM | 13301 | С | VAL | 1979 | | -38.099 | 20.926 | 1.00 | 12.11 |
| | | | | | | | | | |
| ATOM | 13302 | 0 | VAL | 1979 | | -37.274 | 20.637 | 1.00 | 13.15 |
| MOTA | 13303 | N | LEU | 1980 | 23.119 | -39.216 | 20.238 | 1.00 | 12.53 |
| ATOM | 13304 | CA | LEU | 1980 | 23.829 | -39.547 | 19.009 | 1.00 | 14.61 |
| MOTA | 13305 | CB | LEU | 1980 | 24.510 | -40.913 | 19.103 | 1.00 | 16.21 |
| ATOM | 13306 | CG | LEU | 1980 | | -41.049 | 19.799 | 1.00 | 21.32 |
| | | | | | | -42.498 | 19.648 | 1.00 | 17.71 |
| ATOM | 13307 | CD1 | | 1980 | | | | | |
| MOTA | 13308 | CD2 | LEU | 1980 | | -40.094 | 19.170 | 1.00 | 18.47 |
| MOTA | 13309 | С | LEU | 1980 | 22.747 | -39.616 | 17.946 | 1.00 | 15.13 |
| MOTA | 13310 | 0 | LEU | 1980 | 21.812 | -40.411 | 18.060 | 1.00 | 12.67 |
| MOTA | 13311 | N | GLU | 1981 | 22.880 | -38.786 | 16.916 | 1.00 | 14.35 |
| ATOM | 13312 | CA | GLU | 1981 | | -38.726 | 15.851 | 1.00 | 17.03 |
| | | | | | | | | | |
| MOTA | 13313 | CB | GLU | 1981 | | -37.314 | 15.799 | 1.00 | 15.90 |
| MOTA | 13314 | CG | GLU | 1981 | 20.445 | | 14.584 | | 20.75 |
| MOTA | 13315 | CD | GLU | 1981 | 19.621 | -35.740 | 14.747 | 1.00 | 23.90 |
| MOTA | 13316 | OE1 | GLU | 1981 | 20.106 | -34.784 | 15.389 | 1.00 | 25.09 |
| ATOM | 13317. | OE2 | | 1981 | | -35.692 | 14.221 | 1.00 | 26.95 |
| | | C | | 1981 | | -39.120 | 14.479 | 1.00 | 17.13 |
| MOTA | 13318 | | GLU | | | | | | |
| MOTA | 13319 | 0 | GLU | 1981 | | -38.590 | 14.007 | 1.00 | 18.47 |
| ATOM | 13320 | N | CYS | 1982 | 21.733 | -40.065 | 13.849 | 1.00 | 17.94 |
| MOTA | 13321 | CA | CYS | 1982 | 22.080 | -40.532 | 12.513 | 1.00 | 19.05 |
| ATOM | 13322 | CB | CYS | 1982 | 21.599 | -39.505 | 11.489 | 1.00 | 18.86 |
| ATOM | 13323 | SG | CYS | 1982 | 19.782 | | 11.492 | 1.00 | 25.27 |
| | | | | | | | | | 20.26 |
| ATOM | 13324 | C | CYS | 1982 | 23.554 | | 12.313 | | |
| MOTA | 13325 | 0 | CYS | 1982 | 24.276 | | 11.616 | | 21.64 |
| MOTA | 13326 | N | VAL | 1983 | 23.980 - | -41.947 | 12.920 | 1.00 | 21.57 |
| MOTA | 13327 | CA | VAL | 1983 | 25.359 | -42.399 | 12.844 | 1.00 | 22.20 |
| MOTA | 13328 | CB | VAL | 1983 | | -42.075 | 14.172 | 1.00 | 23.68 |
| ATOM | 13329 | | VAL | 1983 | | -42.952 | 15.287 | 1.00 | 24.53 |
| | | | | | | | | | 26.35 |
| MOTA | 13330 | CG2 | | 1983 | | -42.253 | 14.021 | 1.00 | |
| MOTA | 13331 | С | VAL | 1983 | | -43.913 | 12.614 | | 21.11 |
| MOTA | 13332 | 0 | VAL | 1983 | 24.415 | -44.605 | 13.011 | 1.00 | 19.74 |
| MOTA | 13333 | N | PRO | 1984 | 26.382 | -44.450 | 11.945 | 1.00 | 21.78 |
| ATOM | 13334 | CD | PRO | 1984 | | -43.820 | 11.312 | 1.00 | 23.46 |
| | | | | | | -45.898 | 11.724 | 1.00 | 20.82 |
| ATOM | 13335 | CA | PRO | 1984 | | | | | |
| MOTA | 13336 | CB | PRO | 1984 | | -46.130 | 10.992 | | 23.68 |
| ATOM | 13337 | CG | PRO | 1984 | | -44.935 | 11.367 | | 24.78 |
| MOTA | 13338 | С | PRO | 1984 | 26.296 | -46.663 | 13.043 | 1.00 | 18.82 |
| MOTA | 13339 | 0 | PRO | 1984 | | -46.268 | 14.040 | 1.00 | 18.80 |
| ATOM | 13340 | N | VAL | 1985 | | -47.753 | 13.038 | | 18.79 |
| | | | | | | | | | |
| MOTA | 13341 | CA | VAL | 1985 | | -48.578 | 14.225 | | 19.02 |
| MOTA | 13342 | CB | VAL | 1985 | | -49.873 | 13.874 | | 20.60 |
| MOTA | 13343 | CG1 | VAL | 1985 | 24.312 | -50.691 | 15.122 | 1.00 | 20.17 |
| ATOM | 13344 | CG2 | VAL | 1985 | 23.236 - | -49.524 | 13.214 | 1.00 | 17.11 |
| ATOM | 13345 | С | VAL | 1985 | | -48.980 | 14.909 | | 20.44 |
| ATOM | 13346 | o | VAL | | | -48.931 | 16.136 | | 19.37 |
| | | | | 1985 | | | | | |
| ATOM | 13347 | N | GLU | 1986 | | -49.383 | 14.122 | | 20.52 |
| MOTA | 13348 | CA | GLU | 1986 | | -49.800 | 14.692 | | 21.16 |
| MOTA | 13349 | CB | GLU | 1986 | 29.858 - | -50.322 | 13.605 | 1.00 | 23.66 |
| | | | | | | | | | |

| ATOM | 13350 | CG | GLU | 1986 | 29.427 | -50.073 | 12.168 | 1.00 30.18 |
|--------------|----------------|----------|------------|--------------|--------|--------------------|------------------|--------------------------|
| MOTA | 13351 | CD | GLU | 1986 | | -50.765 | 11.822 | 1.00 31.01 |
| MOTA | 13352 | | | 1986 | | -51.957 | 12.162 | 1.00 34.03 |
| MOTA | 13353 | OE2 | GLU | 1986 | | -50.116 | 11.207 | 1.00 32.54 |
| MOTA | 13354 | С | GLU | 1986 | | -48.667 -48.904 | 15.458 16.486 | 1.00 19.79 1.00 20.21 |
| ATOM ATOM | 13355 13356 | O N | GLU LEU | 1986 1987 | | -47.440 | 14.959 | 1.00 20.21 |
| ATOM | 13357 | CA | LEU | 1987 | | -46.288 | 15.629 | 1.00 19.57 |
| ATOM | 13358 | СВ | LEU | 1987 | | -45.039 | 14.743 | 1.00 21.80 |
| MOTA | 13359 | CG | LEU | 1987 | 31.137 | -44.044 | 14.841 | 1.00 24.62 |
| MOTA | 13360 | CD1 | LEU | 1987 | 30.711 | -42.719 | 14.230 | 1.00 24.77 |
| MOTA | 13361 | | LEU | 1987 | | -43.849 | 16.275 | 1.00 27.37 |
| MOTA | 13362 | С | LEU | 1987 | | -46.015 | 16.930 | 1.00 19.16 |
| MOTA | 13363 | 0 | LEU | 1987 | | -45.704 -46.129 | 17.957 16.879 | 1.00 19.07 1.00 17.69 |
| ATOM ATOM | 13364 13365 | N CA | ALA ALA | 1988 1988 | | -45.129 | 18.056 | 1.00 17.03 |
| MOTA | 13366 | CB | ALA | 1988 | | -46.063 | 17.695 | 1.00 18.29 |
| ATOM | 13367 | C | ALA | 1988 | | -46.919 | 19.131 | 1.00 17.28 |
| ATOM | 13368 | 0 | ALA | 1988 | 27.506 | -46.608 | 20.329 | 1.00 15.24 |
| MOTA | 13369 | N | LYS | 1989 | 27.846 | -48.130 | 18.692 | 1.00 18.47 |
| MOTA | 13370 | CA | LYS | 1989 | | -49.203 | 19.598 | 1.00 20.98 |
| ATOM | 13371 | CB | LYS | 1989 | | -50.493 | 18.821 | 1.00 25.15 |
| MOTA | 13372 | CG | LYS | 1989 | | -50.977 -52.169 | 17.875 17.038 | 1.00 30.44 1.00 33.35 |
| ATOM ATOM | 13373 13374 | CD | LYS LYS | 1989 1989 | | -52.561 | 15.968 | 1.00 33.33 |
| MOTA | 13375 | NZ | LYS | 1989 | | -53.556 | 15.000 | 1.00 37.47 |
| MOTA | 13376 | C | LYS | 1989 | | -48.784 | 20.300 | 1.00 19.44 |
| MOTA | 13377 | 0 | LYS | 1989 | 29.656 | -48.853 | 21.523 | 1.00 20.34 |
| MOTA | 13378 | N | ARG | 1990 | | -48.361 | 19.503 | 1.00 18.82 |
| MOTA | 13379 | CA | ARG | 1990 | | -47.951 | 20.017 | 1.00 18.71 |
| ATOM | 13380 | CB | ARG | 1990 | | -47.459 -47.609 | 18.872 | 1.00 23.33 |
| MOTA | 13381 13382 | CG CD | ARG ARG | 1990 1990 | | -47.609 -46.751 | 19.159 18.249 | 1.00 28.11 1.00 31.00 |
| ATOM ATOM | 13383 | NE | ARG | 1990 | | -46.823 | 16.841 | 1.00 31.00 |
| ATOM | 13384 | CZ | ARG | 1990 | | -46.132 | 15.871 | 1.00 34.97 |
| ATOM | 13385 | NH1 | ARG | 1990 | 36.345 | -45.320 | 16.155 | 1.00 34.80 |
| MOTA | 13386 | NH2 | | 1990 | | -46.239 | 14.619 | 1.00 35.67 |
| MOTA | 13387 | С | ARG | 1990 | | -46.848 | 21.058 | 1.00 17.38 |
| ATOM | 13388 | 0 | ARG | 1990 | | -46.901 | 22.125 | 1.00 16.41 |
| MOTA MOTA | 13389 13390 | N CA | ILE ILE | 1991 1991 | | -45.847 -44.718 | 20.744 21.647 | 1.00 15.72 1.00 14.45 |
| ATOM | 13391 | CB | ILE | 1991 | | -43.586 | 20.897 | 1.00 13.43 |
| ATOM | 13392 | CG2 | ILE | 1991 | | -42.468 | 21.887 | 1.00 15.10 |
| ATOM | 13393 | CG1 | ILE | 1991 | 30.797 | -43.074 | 19.767 | 1.00 13.76 |
| MOTA | 13394 | CD1 | | 1991 . | | -41.892 | 18.986 | 1.00 15.99 |
| MOTA | 13395 | С | ILE | 1991 | | -45.087 | 22.933 | 1.00 13.45 |
| MOTA | 13396 | 0 | ILE | 1991 | | -44.674 | 24.029 | 1.00 14.39 1.00 13.96 |
| ATOM ATOM | 13397 13398 | N CA | THR THR | 1992 1992 | | -45.877 -46.288 | 22.799 23.964 | 1.00 13.36 |
| ATOM | 13399 | CB | THR | 1992 | | -47.044 | 23.547 | 1.00 13.12 |
| ATOM | 13400 | OG1 | | 1992 | | -46.196 | 22.708 | 1.00 13.87 |
| MOTA | 13401 | CG2 | THR | 1992 | 25.991 | -47.432 | 24.779 | 1.00 12.06 |
| MOTA | 13402 | С | THR | 1992 | | -47.153 | 24.922 | 1.00 16.80 |
| MOTA | 13403 | 0 | THR | 1992 | | -47.043 -48.007 | 26.142 24.375 | 1.00 15.55 1.00 18.05 |
| ATOM ATOM | 13404 13405 | N CA | GLU GLU | 1993 1993 | | -48.869 | 25.219 | 1.00 18.03 |
| ATOM | 13405 | CB | GLU | 1993 | | -50.069 | 24.413 | 1.00 13.12 |
| ATOM | 13407 | CG | GLU | 1993 | | -50.833 | 23.681 | 1.00 26.97 |
| MOTA | 13408 | CD | GLU | 1993 | 30.495 | -52.105 | 23.018 | 1.00 29.74 |
| MOTA | 13409 | OE1 | | 1993 | | -52.156 | 22.646 | 1.00 32.85 |
| ATOM | 13410 | OE2 | | 1993 | | -53.050 | 22.856 | 1.00 31.62 |
| ATOM | 13411 13412 | C | GLU | 1993 | | -48.077 -48.440 | 25.783 26.814 | 1.00 19.25 1.00 20.28 |
| ATOM ATOM | 13412 | O N | GLU ALA | 1993 1994 | | -46.989 | 25.115 | 1.00 20.28 |
| ATOM | 13414 | CA | ALA | 1994 | | -46.178 | 25.564 | 1.00 18.10 |
| ATOM | 13415 | CB | ALA | 1994 | | -45.383 | 24.398 | 1.00 18.09 |
| MOTA | 13416 | С | ALA | 1994 | | -45.234 | 26.703 | 1.00 18.12 |
| ATOM | 13417 | 0 | ALA | 1994 | | -44.928 | 27.565 | 1.00 19.20 |
| ATOM | 13418 | N | LEU | 1995 | | -44.770 -43.841 | 26.708 | 1.00 17.31 |
| ATOM ATOM | 13419 13420 | CA CB | LEU LEU | 1995 1995 | | -43.841 -42.821 | 27.741 27.145 | 1.00 17.19 1.00 17.68 |
| ATOM | 13421 | CG | LEU | 1995 | | -42.621 | 26.173 | 1.00 17.08 |
| ATOM | 13422 | CD1 | | 1995 | | -40.764 | 25.924 | 1.00 12.73 |
| MOTA | 13423 | CD2 | | 1995 | 31.976 | -41.083 | 26.718 | 1.00 24.11 |
| MOTA | 13424 | С | LEU | 1995 | | -44.507 | 28.924 | 1.00 15.56 |
| MOTA | 13425 | 0 | LEU | 1995 | | -45.496 | 28.766 | 1.00 17.28 |
| MOTA | 13426 | N | ALA | 1996 | 30./39 | -43.942 | 30.106 | 1.00 15.73 |

| MOTA | 13427 | CA | ALA | 1996 | 30.128 | -44.435 | 31.324 | 1.00 15.27 |
|------|-------|----------|--------|------|--------|---------|--------|------------|
| ATOM | 13428 | CB | ALA | 1996 | 30.946 | -44.020 | 32.541 | 1.00 15.65 |
| ATOM | 13429 | С | ALA | 1996 | 28.727 | -43.836 | 31.402 | 1.00 14.70 |
| ATOM | 13430 | Ö | ALA | 1996 | | -44.485 | 31.871 | 1.00 14.43 |
| ATOM | 13431 | N | ILE | 1997 | | -42.595 | 30.934 | 1.00 14.99 |
| | | | | 1997 | | -41.939 | 30.946 | 1.00 13.59 |
| ATOM | 13432 | CA | ILE | | | | | |
| MOTA | 13433 | CB | ILE | 1997 | | -40.419 | 30.633 | 1.00 13.71 |
| MOTA | 13434 | CG2 | ILE | 1997 | | -39.710 | 31.721 | 1.00 10.02 |
| MOTA | 13435 | CG1 | ILE | 1997 | | -40.211 | 29.249 | 1.00 11.88 |
| MOTA | 13436 | CD1 | ILE | 1997 | 28.068 | -38.736 | 28.834 | 1.00 13.96 |
| MOTA | 13437 | С | ILE | 1997 | 26.337 | -42.565 | 29.909 | 1.00 12.60 |
| MOTA | 13438 | 0 | ILE | 1997 | 26.786 | -43.173 | 28.935 | 1.00 12.53 |
| ATOM | 13439 | N | PRO | 1998 | 25.018 | -42.431 | 30.111 | 1.00 13.25 |
| ATOM | 13440 | CD | PRO | 1998 | 24.297 | -41.930 | 31.296 | 1.00 10.70 |
| ATOM | 13441 | CA | PRO | 1998 | | -43.019 | 29.128 | 1.00 12.65 |
| ATOM | 13442 | CB | PRO | 1998 | | -42.952 | 29.824 | 1.00 13.84 |
| ATOM | 13443 | CG | PRO | 1998 | | -41.813 | 30.788 | 1.00 18.97 |
| ATOM | 13444 | C | PRO | 1998 | | -42.292 | 27.784 | 1.00 12.72 |
| | 13445 | 0 | | 1998 | | -41.081 | 27.718 | 1.00 12.72 |
| ATOM | | | PRO | | | -43.053 | 26.721 | 1.00 12.60 |
| ATOM | 13446 | N | VAL | 1999 | | | | |
| ATOM | 13447 | CA | VAL | 1999 | | -42.507 | 25.376 | |
| ATOM | 13448 | CB | VAL | 1999 | | -43.123 | 24.507 | 1.00 14.39 |
| ATOM | 13449 | | VAL | 1999 | | -42.664 | 23.061 | 1.00 13.88 |
| ATOM | 13450 | | VAL | 1999 | | -42.685 | 25.062 | 1.00 13.61 |
| MOTA | 13451 | С | VAL | 1999 | | -42.815 | 24.784 | 1.00 12.68 |
| MOTA | 13452 | 0 | VAL | 1999 | | -43.969 | 24.753 | 1.00 11.67 |
| MOTA | 13453 | N | ILE | 2000 | 21.788 | -41.768 | 24.346 | 1.00 12.00 |
| MOTA | 13454 | CA | ILE | 2000 | 20.449 | -41.870 | 23.772 | 1.00 10.42 |
| MOTA | 13455 | CB | ILE | 2000 | 19.527 | -40.764 | 24.362 | 1.00 11.32 |
| MOTA | 13456 | CG2 | ILE | 2000 | 18.190 | -40.765 | 23.645 | 1.00 14.54 |
| ATOM | 13457 | CG1 | | 2000 | 19.350 | -40.977 | 25.869 | 1.00 12.67 |
| ATOM | 13458 | | ILE | 2000 | | -39.808 | 26.580 | 1.00 14.64 |
| ATOM | 13459 | C | ILE | 2000 | | -41.667 | 22.265 | |
| ATOM | 13460 | ō | ILE | 2000 | | -40.682 | 21.814 | 1.00 12.18 |
| ATOM | 13461 | N | GLY | 2001 | | -42.595 | 21.486 | 1.00 9.93 |
| | | CA | | 2001 | | -42.462 | 20.048 | 1.00 10.42 |
| MOTA | 13462 | | GLY | | | | 19.274 | 1.00 10.42 |
| ATOM | 13463 | С | GLY | 2001 | | -42.223 | | |
| MOTA | 13464 | 0 | GLY | 2001 | | -42.486 | 19.742 | 1.00 10.35 |
| ATOM | 13465 | N | ILE | 2002 | | -41.667 | 18.085 | 1.00 12.38 |
| MOTA | 13466 | CA | ILE | 2002 | | -41.430 | 17.149 | 1.00 12.82 |
| MOTA | 13467 | CB | ILE | 2002 | | -39.975 | 17.254 | 1.00 15.11 |
| MOTA | 13468 | CG2 | ILE | 2002 | | -38.929 | 17.272 | 1.00 17.13 |
| MOTA | 13469 | CG1 | ILE | 2002 | | -39.726 | 16.101 | 1.00 16.48 |
| MOTA | 13470 | CD1 | ILE | 2002 | 15.206 | -40.620 | 16.103 | 1.00 21.78 |
| MOTA | 13471 | C | ILE | 2002 | 18.652 | -41.700 | 15.832 | 1.00 14.25 |
| MOTA | 13472 | 0 | ILE | 2002 | 19.612 | -41.019 | 15.465 | 1.00 14.32 |
| ATOM | 13473 | N | GLY | 2003 | 18.202 | -42.745 | 15.145 | 1.00 13.78 |
| ATOM | 13474 | CA | GLY | 2003 | 18.839 | -43.124 | 13.902 | 1.00 13.18 |
| ATOM | 13475 | С | GLY | 2003 | 20.243 | -43.651 | 14.160 | 1.00 13.92 |
| ATOM | 13476 | 0 | GLY | 2003 | 21.108 | -43.548 | 13.293 | 1.00 16.63 |
| ATOM | 13477 | N | ALA | 2004 | | -44.208 | 15.347 | 1.00 14.85 |
| ATOM | 13478 | CA | ALA | 2004 | | -44.758 | 15.677 | 1.00 15.30 |
| ATOM | 13479 | СВ | ALA | 2004 | | -43.972 | 16.832 | 1.00 16.97 |
| ATOM | 13480 | C | ALA | 2004 | 21.732 | -46.247 | 16.031 | 1.00 15.54 |
| ATOM | 13481 | ō | ALA | 2004 | 22.688 | -46.814 | 16.565 | 1.00 18.51 |
| MOTA | 13482 | N | GLY | 2005 | 20.598 | -46.880 | 15.741 | 1.00 16.16 |
| MOTA | 13483 | CA | GLY | 2005 | 20.448 | -48.302 | 16.033 | 1.00 14.60 |
| | 13484 | | GLY | | • | -48.614 | 17.473 | |
| MOTA | | C | | 2005 | | | | |
| MOTA | 13485 | 0 | GLY | 2005 | 20.022 | -47.717 | 18.311 | 1.00 16.19 |
| ATOM | 13486 | N | ASN | 2006 | 19.843 | -49.891 | 17.773 | 1.00 14.74 |
| ATOM | 13487 | CA | ASN | 2006 | | -50.290 | 19.130 | 1.00 14.82 |
| ATOM | 13488 | CB | ASN | 2006 | | -51.530 | 19.083 | 1.00 14.04 |
| ATOM | 13489 | CG | ASN | 2006 | | -52.803 | 18.712 | 1.00 12.52 |
| MOTA | 13490 | | ASN | 2006 | | -53.901 | 18.870 | 1.00 16.70 |
| MOTA | 13491 | ND2 | ASN | 2006 | | -52.668 | 18.222 | 1.00 12.06 |
| ATOM | 13492 | C | ASN | 2006 | | -50:548 | 20.094 | 1.00 14.16 |
| ATOM | 13493 | 0 | ASN | 2006 | 20.403 | -51.082 | 21.183 | 1.00 15.13 |
| MOTA | 13494 | N | VAL | 2007 | 21.817 | -50.153 | 19.703 | 1.00 14.84 |
| MOTA | 13495 | CA | VAL | 2007 | 23.002 | -50.358 | 20.534 | 1.00 16.00 |
| MOTA | 13496 | CB | VAL | 2007 | | -50.349 | 19.677 | 1.00 18.48 |
| MOTA | 13497 | | VAL | 2007 | | -50.869 | 20.490 | 1.00 25.46 |
| MOTA | 13498 | | VAL | 2007 | | -51.178 | 18.421 | 1.00 22.41 |
| ATOM | 13499 | C | VAL | 2007 | 23.167 | -49.310 | 21.639 | 1.00 16.08 |
| ATOM | 13500 | ō | VAL | 2007 | | -49.486 | 22.557 | 1.00 14.39 |
| ATOM | 13501 | N | THR | 2008 | | -48.215 | 21.549 | 1.00 13.91 |
| MOTA | 13501 | CA | THR | 2008 | | -47.158 | 22.557 | 1.00 13.64 |
| MOTA | 13502 | CB | THR | 2008 | | -45.809 | 21.980 | 1.00 13.04 |
| 011 | ~~~~ | <u> </u> | T 111/ | 2000 | 44.001 | | , | |

| | | | | | | | | - |
|------------------------------|----------------------------------|--------------------|-------------------|----------------------|----------------------------------|-------------------------------|----------------------------|--|
| MOTA | 13504 | OG1 | THR | 2008 | 20.692 | -45.980 | 21.412 | 1.00 13.88 |
| ATOM | 13505 | CG2 | THR | 2008 | 22 941 | -45.303 | 20.901 | 1.00 14.51 |
| | | | | | | | | |
| MOTA | 13506 | С | THR | 2008 | 21.743 | -47.523 | 23.839 | 1.00 13.63 |
| MOTA | 13507 | 0 | THR | 2008 | 20.956 | -48.470 | 23.847 | 1.00 15.42 |
| MOTA | 13508 | N | ASP | 2009 | 21.993 | -46.796 | 24.925 | 1.00 13.00 |
| | 13509 | CA | ASP | 2009 | | -47.071 | 26.205 | 1.00 12.92 |
| ATOM | | | | | | | | |
| MOTA | 13510 | CB | ASP | 2009 | - | -46.350 | 27.337 | 1.00 13.27 |
| MOTA | 13511 | CG | ASP | 2009 | 23.552 | -46.681 | 27.365 | 1.00 14.17 |
| ATOM | 13512 | | ASP | 2009 | 23 898 | -47.849 | 27.650 | 1.00 15.47 |
| | | | | | | | | |
| MOTA | 13513 | OD2 | ASP | 2009 | 24.362 | -45.779 | 27.093 | 1.00 14.16 |
| MOTA | 13514 | С | ASP | 2009 | 19.859 | -46.652 | 26.208 | 1.00 13.92 |
| MOTA | 13515 | 0 | ASP | 2009 | 19.035 | -47.205 | 26.943 | 1.00 14.59 |
| | 13516 | N | GLY | 2010 | | -45.658 | 25.387 | 1.00 14.50 |
| MOTA | | | | | | | | |
| MOTA | 13517 | CA | GLY | 2010 | 18.173 | | 25.300 | 1.00 13.29 |
| MOTA | 13518 | С | GLY | 2010 | 17.829 | -44.764 | 23.878 | 1.00 11.32 |
| ATOM | 13519 | 0 | GLY | 2010 | 18 700 | -44.728 | 23.008 | 1.00 11.26 |
| | | | | | | | | |
| MOTA | 13520 | N | GLN | 2011 | 16.562 | -44.437 | 23.644 | |
| MOTA | 13521 | CA | GLN | 2011 | 16.095 | -44.032 | 22.325 | 1.00 10.95 |
| ATOM | 13522 | CB | GLN | 2011 | 15.215 | -45.121 | 21.706 | 1.00 12.17 |
| | | | | 2011 | | -46.426 | 21.378 | 1.00 10.38 |
| MOTA | 13523 | CG | GLN | | | | | |
| MOTA | 13524 | CD | GLN | 2011 | 16.987 | -46.262 | 20.303 | 1.00 9.79 |
| ATOM | 13525 | OE1 | GLN | 2011 | 16.812 | -45.508 | 19.344 | 1.00 12.91 |
| MOTA | 13526 | NE2 | GLN | 2011 | 18 086 | -46.986 | 20.445 | 1.00 12.26 |
| | | | | | 15.254 | | | |
| MOTA | 13527 | C | GLN | 2011 | | | 22.417 | |
| MOTA | 13528 | 0 | GLN | 2011 | 14.646 | -42.495 | 23.451 | 1.00 9.84 |
| MOTA | 13529 | N | ILE | 2012 | 15.208 | -42.023 | 21.327 | 1.00 13.12 |
| | 13530 | CA | ILE | 2012 | | -40.835 | 21.307 | 1.00 16.32 |
| MOTA | | | | | | | | |
| MOTA | 13531 | CB | ILE | 2012 | 15.228 | -39.563 | 21.592 | 1.00 20.21 |
| MOTA | 13532 | CG2 | ILE | 2012 | 16.164 | -39.278 | 20.451 | 1.00 19.95 |
| MOTA | 13533 | CG1 | ILE | 2012 | | -38.372 | 21.851 | 1.00 22.75 |
| | | | | | | | | |
| MOTA | 13534 | | ILE | 2012 | 14.955 | -37.275 | 22.672 | 1.00 20.84 |
| MOTA | 13535 | C | ILE | 2012 | 13.700 | -40.764 | 19.951 | 1.00 18.75 |
| MOTA | 13536 | 0 | ILE | 2012 | 14.243 | -41.208 | 18.939 | 1.00 17.43 |
| | 13537 | N | ĽEU | 2013 | | -40.250 | 19.942 | 1.00 19.42 |
| MOTA | | | | | | | | |
| MOTA | 13538 | CA | LEU | 2013 | 11.746 | -40.110 | 18.700 | 1.00 23.65 |
| MOTA | 13539 | CB | LEU | 2013 | 10.914 | -41.356 | 18.419 | 1.00 26.87 |
| ATOM | 13540 | CG | LEU | 2013 | 11 228 | -42.102 | 17.114 | 1.00 28.56 |
| | | | | | | | | |
| MOTA | 13541 | | LEU | 2013 | | -43.189 | 16.952 | 1.00 27.78 |
| MOTA | 13542 | CD2 | LEU | 2013 | 11.206 | -41.148 | 15.900 | 1.00 28.97 |
| MOTA | 13543 | С | LEU | 2013 | 10.835 | -38.903 | 18.751 | 1.00 24.10 |
| | 13544 | ō | LEU | 2013 | | -38.489 | 19.830 | 1.00 19.94 |
| MOTA | | | | | | | | |
| MOTA | 13545 | N | VAL | 2014 | | -38.337 | 17.573 | 1.00 23.42 |
| MOTA | 13546 | CA | VAL | 2014 | 9.714 | -37.186 | 17.420 | 1.00 22.95 |
| MOTA | 13547 | CB | VAL | 2014 | | -36.500 | 16.039 | 1.00 25.08 |
| | | - | | | | | | |
| MOTA | 13548 | CG1 | VAL | 2014 | | -35.340 | 15.907 | 1.00 25.84 |
| MOTA | 13549 | CG2 | VAL | 2014 | 11.312 | -35.989 | 15.898 | 1.00 29.40 |
| ATOM | 13550 | С | VAL | 2014 | 8.310 | -37.732 | 17.499 | 1.00 19.50 |
| ATOM | | | VAL | 2014 | | -38.578 | 16.688 | 1.00 17.37 |
| | 13551 | О | | | | | | |
| ATOM | 13552 | N | MET | 2015 | 7.563 | -37.258 | 18.488 | 1.00 16.88 |
| ATOM | 13553 | CA | MET | 2015 | 6.199 | -37.712 | 18.687 | 1.00 15.75 |
| ATOM | 13554 | CB | MET | 2015 | 5 567 | -37.024 | 19.913 | 1.00 13.34 |
| | | | | | | | | |
| MOTA | 13555 | CG | MET | 2015 | | -35.519 | 19.841 | 1.00 14.95 |
| ATOM | 13556 | SD | MET | 2015 | 3.933 | -34.982 | 20.657 | 1.00 14.22 |
| MOTA | 13557 | CE | MET | 2015 | 2.778 | -35.272 | 19.370 | 1.00 13.27 |
| ATOM | 13558 | C | MET | 2015 | | -37.485 | 17.451 | 1.00 15.30 |
| | | | | | | | | |
| MOTA | 13559 | 0 | MET | 2015 | | -38.288 | 17.150 | 1.00 16.99 |
| ATOM | 13560 | N | HIS | 2016 | | -36.411 | 16.714 | 1.00 12.72 |
| ATOM | 13561 | CA | HIS | 2016 | 4.804 | -36.144 | 15.527 | 1.00 15.08 |
| ATOM | 13562 | CB | HIS | 2016 | | -34.739 | 15.005 | 1.00 15.69 |
| | | | | | | | | |
| MOTA | 13563 | CG | HIS | 2016 | 4.605 | -33.664 | 15.915 | 1.00 14.26 |
| MOTA | 13564 | CD2 | HIS | 2016 | 5.132 | -33.129 | 17.043 | 1.00 11.38 |
| MOTA | 13565 | ND1 | HIS | 2016 | 3.330 | -33.146 | 15.808 | 1.00 15.21 |
| MOTA | 13566 | | HIS | 2016 | | -32.345 | 16.833 | 1.00 13.82 |
| | | | | | | | | |
| MOTA | 13567 | | HIS | 2016 | | -32.318 | 17.598 | 1.00 16.57 |
| MOTA | 13568 | С | HIS | 2016 | 4.989 | -37.221 | 14.462 | 1.00 16.85 |
| MOTA | 13569 | 0 | HIS | 2016 | 4.085 | -37.462 | 13.658 | 1.00 17.99 |
| | | | | 2017 | 6.143 | -37.883 | 14.455 | 1.00 17.44 |
| MOTA | 13570 | N | ASP | | | | | |
| MOTA | 13571 | CA | ASP | 2017 | 6.359 | -38.967 | 13.495 | 1.00 22.03 |
| ATOM | 13572 | CB | ASP | 2017 | 7.850 | -39.142 | 13.177 | 1.00 23.41 |
| ATOM | 13573 | CG | ASP | 2017 | 8.440 | -37.954 | 12.431 | 1.00 27.95 |
| | | | | | | | | |
| MOTA | 12574 | 1 11 1 | ASP | 2017 | 7.857 | -37.548 | 11.409 | 1.00 27.29 |
| | 13574 | | | | 9.488 | -37.442 | 12.873 | |
| ATOM | 13574 13575 | | ASP | 2017 | 3.400 | 37.332 | | 1.00 26.63 |
| MOTA | 13575 | OD2 | | | 5.817 | -40.278 | 14.079 | 1.00 26.63 |
| ATOM ATOM | 13575 13576 | OD2 C | ASP | 2017 | 5.817 | -40.278 | 14.079 | 1.00 21.90 |
| MOTA MOTA MOTA | 13575 13576 13577 | OD2 C O | ASP ASP | 2017 2017 | 5.817 5.254 | -40.278 -41.105 | 14.079 13.357 | 1.00 21.90 1.00 23.38 |
| ATOM ATOM ATOM ATOM | 13575 13576 13577 13578 | OD2 C | ASP | 2017 | 5.817 5.254 5.986 | -40.278 -41.105 -40.454 | 14.079 13.357 15.388 | 1.00 21.90 1.00 23.38 1.00 22.26 |
| MOTA MOTA MOTA | 13575 13576 13577 13578 | OD2 C O | ASP ASP | 2017 2017 2018 | 5.817 5.254 5.986 | -40.278 -41.105 | 14.079 13.357 | 1.00 21.90 1.00 23.38 |
| ATOM ATOM ATOM ATOM | 13575 13576 13577 | OD2 C O N | ASP ASP ALA | 2017 2017 | 5.817 5.254 5.986 5.538 | -40.278 -41.105 -40.454 | 14.079 13.357 15.388 | 1.00 21.90 1.00 23.38 1.00 22.26 |

| MOTA | 13581 | С | ALA | 2018 | 4.037 | -41.923 | 15.959 | 1.00 24.21 |
|--------|-------|-----|------|------|--------|---------|--------|------------|
| MOTA | 13582 | 0 | ALA | 2018 | 3.597 | -43.064 | 16.085 | 1.00 25.32 |
| ATOM | 13583 | N | PHE | 2019 | 3.255 | -40.871 | 15.711 | 1.00 21.91 |
| | 13584 | CA | PHE | 2019 | 1.807 | -41.011 | 15.561 | 1.00 22.15 |
| MOTA | | | | | 1.080 | -40.151 | 16.596 | 1.00 22.13 |
| MOTA | 13585 | CB | PHE | 2019 | | | | |
| MOTA | 13586 | CG | PHE | 2019 | 1.580 | -40.355 | 17.999 | 1.00 24.13 |
| MOTA | 13587 | CD1 | PHE | 2019 | 1.717 | -41.638 | 18.516 | 1.00 24.21 |
| MOTA | 13588 | CD2 | PHE | 2019 | 1.935 | -39.271 | 18.795 | 1.00 25.21 |
| MOTA | 13589 | CE1 | PHE | 2019 | 2.207 | -41.843 | 19.807 | 1.00 25.08 |
| ATOM | 13590 | CE2 | PHE | 2019 | 2.426 | -39.463 | 20.091 | 1.00 25.89 |
| ATOM | 13591 | CZ | PHE | 2019 | 2.561 | -40.752 | 20.593 | 1.00 26.24 |
| | 13592 | C | PHE | 2019 | 1.329 | -40.637 | 14.155 | 1.00 21.96 |
| MOTA | | | | | | | | |
| MOTA | 13593 | 0 | PHE | 2019 | 0.156 | -40.325 | 13.947 | 1.00 22.51 |
| MOTA | 13594 | N | GLY | 2020 | 2.243 | -40.658 | 13.194 | 1.00 23.05 |
| MOTA | 13595 | CA | GLY | 2020 | 1.879 | -40.328 | 11.829 | 1.00 24.29 |
| MOTA | 13596 | C | GLY | 2020 | 1.192 | -38.985 | 11.660 | 1.00 23.30 |
| MOTA | 13597 | 0 | GLY | 2020 | 0.433 | -38.791 | 10.706 | 1.00 24.31 |
| ATOM | 13598 | N | ILE | 2021 | 1.445 | -38.049 | 12.570 | 1.00 22.12 |
| ATOM | 13599 | CA | ILE | 2021 | 0.822 | -36.731 | 12.466 | 1.00 19.93 |
| | | | | 2021 | 0.976 | -35.919 | 13.792 | 1.00 18.55 |
| ATOM | 13600 | CB | ILE | | | | | |
| MOTA | 13601 | CG2 | ILE | 2021 | 0.483 | -34.500 | 13.595 | 1.00 18.65 |
| MOTA | 13602 | CG1 | ILE | 2021 | 0.168 | -36.590 | 14.912 | 1.00 17.73 |
| MOTA | 13603 | CD1 | ILE | 2021 | 0.485 | -36.084 | 16.319 | 1.00 15.80 |
| MOTA | 13604 | С | ILE | 2021 | 1.447 | -35.961 | 11.300 | 1.00 20.77 |
| MOTA | 13605 | 0 | ILE | 2021 | 0.738 | -35.348 | 10.502 | 1.00 18.99 |
| ATOM | 13606 | N | THR | 2022 | 2.771 | -36.008 | 11.194 | 1.00 22.40 |
| ATOM | | ·CA | THR | 2022 | | -35.313 | 10.120 | 1.00 25.87 |
| ATOM | 13608 | | THR | 2022 | | -35.269 | 10.385 | 1.00 27.00 |
| | | CB | | | | | | |
| MOTA | 13609 | OG1 | THR | 2022 | | -36.600 | 10.373 | 1.00 32.73 |
| MOTA | 13610 | CG2 | THR | 2022 | | -34.641 | 11.735 | 1.00 26.74 |
| MOTA | 13611 | С | THR | 2022 | 3.240 | -35.978 | 8.765 | 1.00 27.71 |
| ATOM | 13612 | 0 | THR | 2022 | 3.208 | -37.208 | 8.663 | 1.00 26.18 |
| MOTA | 13613 | N | GLY | 2023 | 3.078 | -35.147 | 7.738 | 1.00 29.75 |
| ATOM | 13614 | CA | GLY | 2023 | | -35.620 | 6.381 | 1.00 36.68 |
| ATOM | 13615 | C | GLY | 2023 | 2.624 | -37.111 | 6.213 | 1.00 40.05 |
| | | | GLY | 2023 | | -37.666 | 6.754 | 1.00 41.97 |
| ATOM | 13616 | 0 | | | | | | |
| ATOM | 13617 | N | GLY | 2024 | 3.503 | -37.765 | 5.458 | 1.00 41.61 |
| MOTA | 13618 | CA | GLY | 2024 | | -39.194 | 5.240 | 1.00 43.00 |
| MOTA | 13619 | С | GLY | 2024 | 4.675 | -39.899 | 4.961 | 1.00 43.33 |
| MOTA | 13620 | 0 | GLY | 2024 | 4.750 | -41.125 | 5.012 | 1.00 44.64 |
| MOTA | 13621 | N | HIS | 2025 | 5.712 | -39.125 | 4.664 | 1.00 42.93 |
| ATOM | 13622 | CA | HIS | 2025 | 7.031 | -39.680 | 4.374 | 1.00 42.66 |
| ATOM | 13623 | CB | HIS | 2025 | 7.622 | -38.976 | 3.151 | 1.00 46.48 |
| MOTA | 13624 | CG | HIS | 2025 | 7.432 | -37.489 | 3.161 | 1.00 50.68 |
| | | | | | | | | |
| MOTA | 13625 | | HIS | 2025 | | -36.676 | 2.337 | |
| MOTA | 13626 | | HIS. | 2025 | 8.001 | -36.669 | 4.112 | 1.00 52.20 |
| ATOM . | 13627 | CE1 | HIS | 2025 | 7.660 | -35.415 | 3.872 | 1.00 52.74 |
| MOTA | 13628 | NE2 | HIS | 2025 | 6.888 | -35.392 | 2.801 | 1.00 53.69 |
| ATOM | 13629 | С | HIS | 2025 | 7.983 | -39.548 | 5.563 | 1.00 39.08 |
| MOTA | 13630 | 0 | HIS | 2025 | 8.882 | -38.709 | 5.552 | 1.00 38.93 |
| ATOM | 13631 | N | ILE | 2026 | 7.790 | -40.381 | 6.582 | 1.00 35.71 |
| ATOM | 13632 | CA | ILE | 2026 | | -40.330 | 7.771 | 1.00 32.13 |
| | | | | 2026 | 8.040 | -41.148 | 8.927 | 1.00 33.92 |
| ATOM | 13633 | CB | ILE | | | | | 1 00 35.52 |
| ATOM | 13634 | | ILE | 2026 | | -40.599 | 9.305 | 1.00 35.60 |
| MOTA | 13635 | CG1 | ILE | 2026 | 7.952 | -42.620 | 8.522 | 1.00 33.22 |
| MOTA | 13636 | CD1 | ILE | 2026 | | -43.554 | 9.685 | 1.00 34.59 |
| MOTA | 13637 | C | ILE | 2026 | 10.045 | -40.857 | 7.509 | 1.00 27.67 |
| MOTA | 13638 | 0 | ILE | 2026 | 10.252 | -41.720 | 6.652 | 1.00 27.84 |
| MOTA | 13639 | N | PRO | 2027 | 11.035 | -40.346 | 8.256 | 1.00 25.23 |
| ATOM | 13640 | CD | PRO | 2027 | 10.945 | -39.349 | 9.333 | 1.00 23.72 |
| ATOM | 13641 | CA | PRO | 2027 | | -40.793 | 8.075 | 1.00 23.00 |
| | | | PRO | | | -39.972 | 9.111 | 1.00 24.44 |
| ATOM | 13642 | CB | | 2027 | | | | |
| MOTA | 13643 | CG | PRO | 2027 | | -39.676 | 10.159 | 1.00 26.02 |
| MOTA | 13644 | C | PRO | 2027 | | -42.299 | 8.266 | 1.00 21.46 |
| MOTA | 13645 | 0 | PRO | 2027 | | -42.950 | 8.964 | 1.00 18.01 |
| MOTA | 13646 | N | LYS | 2028 | 13.638 | -42.840 | 7.642 | 1.00 21.15 |
| ATOM | 13647 | CA | LYS | 2028 | 13.928 | -44.266 | 7.722 | 1.00 22.60 |
| ATOM | 13648 | CB | LYS | 2028 | | -44.607 | 6.914 | 1.00 25.69 |
| ATOM | 13649 | CG | LYS | 2028 | | -44.928 | 5.441 | 1.00 33.29 |
| ATOM | 13650 | CD | LYS | 2028 | 14.455 | -43.717 | 4.653 | 1.00 36.85 |
| | | | | | | -44.047 | 3.170 | 1.00 40.01 |
| MOTA | 13651 | CE | LYS | 2028 | | | | |
| ATOM | 13652 | NZ | LYS | 2028 | 14.001 | -42.848 | 2.343 | 1.00 41.13 |
| ATOM | 13653 | С | LYS | 2028 | | -44.767 | 9.146 | 1.00 20.12 |
| MOTA | 13654 | 0 | LYS | 2028 | | -45.901 | 9.448 | 1.00 19.79 |
| MOTA | 13655 | N | PHE | 2029 | | -43.926 | 10.020 | 1.00 18.98 |
| MOTA | 13656 | CA | PHE | 2029 | 14.904 | -44.337 | 11.400 | 1.00 17.08 |
| MOTA | 13657 | CB | PHE | 2029 | 16.031 | -43.494 | 11.994 | 1.00 16.61 |

| ATOM | 13658 | CG | PHE | 2029 | 15.756 | -42.027 | 11.973 | 1.00 18.88 |
|--------|----------------|---------|------------|--------------|--------|--------------------|------------------|--------------------------|
| ATOM | 13659 | CD1 | | 2029 | | -41.459 | 12.882 | 1.00 18.51 |
| ATOM | 13660 | CD2 | PHE | 2029 | 16.353 | -41.211 | 11.014 | 1.00 18.71 |
| ATOM | 13661 | | PHE | 2029 | 14.585 | -40.097 | 12.842 | 1.00 19.42 |
| ATOM | 13662 | CE2 | PHE | 2029 | 16.072 | -39.846 | 10.961 | 1.00 19.33 |
| ATOM | 13663 | CZ | PHE | 2029 | 15.187 | -39.288 | 11.875 | 1.00 19.51 |
| ATOM . | | C | PHE | 2029 | | -44.279 | 12.313 | 1.00 14.56 |
| ATOM | 13665 | ō | PHE | 2029 | 13.732 | -44.765 | 13.435 | 1.00 12.75 |
| ATOM | 13666 | N | ALA | 2030 | 12.587 | -43.706 | 11.822 | 1.00 13.77 |
| ATOM | 13667 | CA | ALA | 2030 | 11.374 | -43.579 | 12.615 | 1.00 13.91 |
| ATOM | 13668 | CB | ALA | 2030 | 10.752 | -42.221 | 12.387 | 1.00 14.25 |
| ATOM | 13669 | C | ALA | 2030 | | -44.661 | 12.345 | 1.00 15.51 |
| ATOM | 13670 | Õ | ALA | 2030 | | -45.389 | 11.356 | 1.00 14.24 |
| ATOM | 13671 | N | LYS | 2031 | | -44.751 | 13.243 | 1.00 13.26 |
| ATOM | 13672 | CA | LYS | 2031 | 8.287 | -45.713 | 13.122 | 1.00 13.53 |
| ATOM | 13673 | CB | LYS | 2031 | 8.599 | -46.980 | 13.924 | 1.00 13.73 |
| ATOM | 13674 | CG | LYS | 2031 | | -48.008 | 13.894 | 1.00 13.98 |
| MOTA | 13675 | CD | LYS | 2031 | 7.871 | -49.321 | 14.566 | 1.00 15.44 |
| ATOM | 13676 | CE | LYS | 2031 | | -50.206 | 14.782 | 1.00 17.20 |
| ATOM | 13677 | NZ | LYS | 2031 | | -51.532 | 15.354 | 1.00 18.85 |
| ATOM | 13678 | C | LYS | 2031 | | -45.096 | 13.625 | 1.00 13.24 |
| ATOM | 13679 | 0 | LYS | 2031 | 6.981 | -44.383 | 14.633 | 1.00 12.44 |
| ATOM | 13680 | N | ASN | 2032 | | -45.359 | 12.900 | 1.00 13.87 |
| ATOM | 13681 | CA | ASN | 2032 | | -44.866 | 13.272 | 1.00 14.13 |
| ATOM | 13682 | СВ | ASN | 2032 | | -44.625 | 12.015 | 1.00 15.58 |
| ATOM | 13683 | CG | ASN | 2032 | | -44.218 | 12.336 | 1.00 17.14 |
| ATOM | 13684 | | ASN | 2032 | | -44.384 | 13.465 | 1.00 18.37 |
| ATOM | 13685 | | ASN | 2032 | | -43.699 | 11.338 | 1.00 15.68 |
| MOTA | 13686 | С | ASN | 2032 | | -45.964 | 14.124 | 1.00 14.09 |
| ATOM | 13687 | 0 | ASN | 2032 | | -46.987 | 13.594 | 1.00 13.04 |
| ATOM | 13688 | N | PHE | 2033 | | -45.760 | 15.435 | 1.00 11.21 |
| ATOM | 13689 | CA | PHE | 2033 | 3.382 | -46.733 | 16.370 | 1.00 13.08 |
| ATOM | 13690 | CB | PHE | 2033 | 3.967 | -46.540 | 17.778 | 1.00 13.19 |
| ATOM | 13691 | CG | PHE | 2033 | 5.412 | -46.946 | 17.888 | 1.00 13.28 |
| ATOM | 13692 | | PHE | 2033 | | -46.051 | 17.569 | 1.00 13.02 |
| MOTA | 13693 | | PHE | 2033 | | -48.254 | 18.240 | 1.00 12.37 |
| ATOM | 13694 | | PHE | 2033 | 7.773 | -46.446 | 17.587 | 1.00 14.04 |
| ATOM | 13695 | CE2 | | 2033 | 7.091 | -48.663 | 18.262 | 1.00 11.80 |
| MOTA | 13696 | CZ | PHE | 2033 | 8.106 | -47.756 | 17.934 | 1.00 12.01 |
| MOTA | 13697 | С | PHE | 2033 | 1.864 | -46.643 | 16.421 | 1.00 14.14 |
| MOTA | 13698 | 0 | PHE | 2033 | 1.183 | -47.603 | 16.788 | 1.00 15.64 |
| MOTA | 13699 | N | LEU | 2034 | 1.315 | -45.493 | 16.054 | 1.00 13.12 |
| MOTA | 13700 | CA | LEU | 2034 | -0.135 | -45.372 | 16.075 | 1.00 14.61 |
| MOTA | 13701 | CB | LEU | 2034 | -0.566 | -43.933 | 15.780 | 1.00 15.30 |
| MOTA | 13702 | CG | LEU | 2034 | -2.088 | -43.744 | 15.737 | 1.00 15.00 |
| MOTA | 13703 | CD1 | LEU | 2034 | -2.712 | -44.235 | 17.047 | 1.00 17.20 |
| MOTA | 13704 | CD2 | LEU | 2034 | -2.419 | -42.283 | 15.484 | 1.00 15.32 |
| MOTA | 13705 | С | LEU | 2034 | -0.741 | -46.331 | 15.039 | 1.00 16.57 |
| MOTA | 13706 | 0 | LEU | 2034 | | -47.004 | 15.313 | 1.00 14.84 |
| ATOM | 13707 | N | ALA | 2035 | | -46.390 | 13.858 | 1.00 20.33 |
| MOTA | 13708 | CA | ALA | 2035 | | -47.266 | 12.783 | 1.00 27.79 |
| MOTA | 13709 | CB | ALA | 2035 | | -47.238 | 11.614 | |
| MOTA | 13710 | С | ALA | 2035 | | -48.700 | 13.269 | 1.00 33.38 |
| ATOM | 13711 | 0 | ALA | 2035 | | -49.483 | 12.664 | 1.00 36.55 |
| MOTA | 13712 | N | GLU | 2036 | | -49.036 | 14.366 | 1.00 37.14 |
| MOTA | 13713 | CA | GLU | 2036 | | -50.373 | 14.954 | 1.00 41.95 |
| MOTA | 13714 | CB | GLU | 2036 | | -50.541 | 16.026 | 1.00 42.91 |
| MOTA | 13715 | CG | GLU | 2036 | | -50.150 | 15.573 | 1.00 47.48 |
| MOTA | 13716 | CD | GLU | 2036 | | -51.058 | 14.493 | 1.00 49.09 |
| MOTA | 13717 | | GLU | 2036 | | -50.704 | 13.909 | 1.00 50.73 |
| MOTA | 13718 | | GLU | 2036 | | -52.125 | 14.231 | 1.00 51.86 |
| MOTA | 13719 | С | GLU | 2036 | | -50.605 | 15.591 | 1.00 43.11 |
| MOTA | 13720 | 0 | GLU | 2036 | | -51.740 | 15.916 | 1.00 44.60 |
| ATOM | 13721 | N | THR | 2037 | -2.313 | -49.520 | 15.770 | 1.00 43.75 |
| ATOM | 13722 | CA | THR | 2037 | | -49.569 | 16.372 | 1.00 43.51 |
| MOTA | 13723 | CB | THR | 2037 | -3.554 | -49.742 | 17.894 | 1.00 44.86 |
| ATOM | 13724 | 0G1 | | | | -49.832 | 18.452 | 1.00 46.90 |
| ATOM | 13725 | | THR | 2037 | | -48.567 | 18.513 | 1.00 47.17 |
| ATOM | 13726 | C | THR | 2037 | | -48.283 | 16.075 | 1.00 41.90 |
| ATOM | 13727 | O N | THR | 2037 | | -47.644 -47.916 | 15.046 | 1.00 43.72 |
| MOTA | 13728 | N | GLY | 2038 | | -47.916 -46.700 | 16.976 16.809 | 1.00 38.86 1.00 32.91 |
| ATOM | 13729 | CA | GLY | 2038 | | | | |
| ATOM | 13730 | C | GLY | 2038 | | -45.946 | 18.123 | 1.00 29.01 1.00 29.97 |
| MOTA | 13731 | O N | GLY | 2038 | | -45.193 -46.157 | 18.383 18.964 | 1.00 23.77 |
| ATOM . | 13732 13733 | N CA | ASP ASP | 2039 2039 | | -45.510 | 20.271 | 1.00 23.77 |
| ATOM . | 13734 | CB | ASP | 2039 | | -46.503 | 21.353 | 1.00 23.10 |
| 011 | T 2 , 2 4 | -2 | | 2000 | 3.554 | | | |

| ATOM | 13735 | CG | ASP | 2039 | -5.458 -45.935 | 22.755 | 1.00 | 26.45 |
|--|--|---|---|--|--|--|--|--|
| MOTA | 13736 | | ASP | 2039 | -4.352 -45.993 | 23.316 | | 25.80 |
| ATOM | 13737 | | ASP | 2039 | -6.466 -45.412 | 23.284 | | 33.68 |
| ATOM | 13738 | C | ASP | 2039 | -3.709 -45.026 | 20.528 | | 15.18 |
| ATOM | 13739 | ō | ASP | 2039 | -2.770 -45.814 | 20.510 | 1.00 | |
| ATOM | 13740 | N | ILE | 2040 | -3.562 -43.725 | 20.762 | 1.00 | |
| ATOM | 13741 | CA | ILE | 2040 | -2.256 -43.121 | 20.989 | 1.00 | |
| ATOM | 13742 | CB | ILE | 2040 | -2.379 -41.579 | 21.053 | 1.00 | |
| ATOM | 13742 | CG2 | ILE | 2040 | -1.046 -40.954 | 21.421 | 1.00 | |
| ATOM | 13744 | CG1 | ILE | 2040 | -2.842 -41.052 | 19.689 | 1.00 | |
| ATOM | 13745 | CD1 | ILE | 2040 | -3.192 -39.555 | 19.673 | 1.00 | |
| ATOM | 13746 | C | ILE | 2040 | -1.544 -43.645 | 22.234 | 1.00 | |
| ATOM | 13747 | ō | ILE | 2040 | -0.336 -43.838 | 22.214 | 1.00 | |
| ATOM | 13748 | N | ARG | 2041 | -2.280 -43.881 | 23.312 | 1.00 | |
| ATOM | 13749 | CA | ARG | 2041 | -1.657 -44.390 | 24.520 | 1.00 | |
| ATOM | 13750 | CB | ARG | 2041 | -2.667 -44.389 | 25.660 | 1.00 | |
| ATOM | 13751 | CG | ARG | 2041 | -2.981 -42.985 | 26.125 | 1.00 | |
| ATOM | 13752 | CD | ARG | 2041 | -4.050 -42.968 | 27.178 | 1.00 | |
| ATOM | 13753 | NE | ARG | 2041 | -4.194 -41.629 | 27.733 | 1.00 | |
| ATOM | 13754 | CZ | ARG | 2041 | -4.651 -40.579 | 27.057 | 1.00 | |
| ATOM | 13755 | NH1 | ARG | 2041 | -5.024 -40.700 | 25.791 | 1.00 | |
| ATOM | 13756 | NH2 | ARG | 2041 | -4.728 -39.397 | 27.646 | 1.00 | |
| ATOM | 13757 | С | ARG | 2041 | -1.113 -45.793 | 24.264 | 1.00 | 12.55 |
| ATOM | 13758 | ō | ARG | 2041 | -0.026 -46.143 | 24.729 | 1.00 | |
| ATOM | 13759 | N | ALA | 2042 | -1.862 -46.598 | 23.515 | 1.00 | |
| ATOM | 13760 | CA | ALA | 2042 | -1.405 -47.946 | 23.186 | 1.00 | |
| ATOM | 13761 | CB | ALA | 2042 | -2.481 -48.698 | 22.387 | 1.00 | |
| ATOM | 13762 | C | ALA | 2042 | -0.115 -47.838 | 22.368 | 1.00 | |
| ATOM | 13763 | Ō | ALA | 2042 | 0.823 -48.625 | 22.554 | 1.00 | 13.69 |
| ATOM | 13764 | N | ALA | 2043 | -0.068 -46.862 | 21.462 | 1.00 | 11.53 |
| ATOM | 13765 | CA | ALA | 2043 | 1.121 -46.648 | 20.629 | 1.00 | 11.50 |
| ATOM | 13766 | CB | ALA | 2043 | 0.863 -45.552 | 19.605 | 1.00 | 10.75 |
| ATOM | 13767 | С | ALA | 2043 | 2.322 -46.277 | 21.491 | 1.00 | 10.66 |
| ATOM | 13768 | 0 | ALA | 2043 | 3.439 -46.727 | 21.235 | 1.00 | 12.15 |
| ATOM | 13769 | N | VAL | 2044 | 2.093 -45.449 | 22.505 | 1.00 | 9.56 |
| ATOM | 13770 | CA | VAL | 2044 | 3.166 -45.060 | 23.410 | 1.00 | 9.69 |
| ATOM | 13771 | CB | VAL | 2044 | 2.684 -43.988 | 24.419 | 1.00 | 11.94 |
| ATOM | 13772 | CG1 | VAL | 2044 | 3.702 -43.828 | 25.536 | 1.00 | 11.70 |
| ATOM | 13773 | CG2 | VAL | 2044 | 2.506 -42.656 | 23.694 | 1.00 | 9.79 |
| ATOM | 13774 | С | VAL | 2044 | 3.695 -46.278 | 24.163 | 1.00 | 11.89 |
| ATOM | 13775 | 0 | VAL | 2044 | 4.910 -46.478 | 24.268 | 1.00 | 11.33 |
| MOTA | 13776 | N | ARG | 2045 | 2.782 -47.101 | 24.672 | 1.00 | 10.73 |
| ATOM | 13777 | CA | ARG | 2045 | 3.178 -48.301 | 25.409 | 1.00 | 12.45 |
| ATOM | 13778 | CB | ARG | 2045 | 1.939 -49.016 | 25.956 | 1.00 | 11.81 |
| ATOM | 13779 | CG | ARG | 2045 | 1.325 -48.297 | 27.150 | 1.00 | 15.71 |
| MOTA | 13780 | CD | ARG | 2045 | 0.359 -49.185 | 27.908 | 1.00 | 17.80 |
| MOTA | | CD | _ | 2045 | -0.791 -49.608 | | | |
| 3 0001 | 13781 | NE | ARG | 2045 | | 27.115 | 1.00 | |
| ATOM | 13781 13782 | | ARG ARG | 2045 | -1.866 -48.862 | 27.115 26.874 | 1.00 | 19.90 |
| ATOM | | NE CZ | | | -1.955 -47.632 | 26.874 27.360 | 1.00 1.00 | 19.90 18.74 |
| | 13782 | NE CZ | ARG | 2045 | -1.955 -47.632 -2.874 -49.358 | 26.874 27.360 26.165 | 1.00 1.00 1.00 | 19.90 18.74 17.78 |
| MOTA | 13782 13783 | NE CZ NH1 | ARG ARG | 2045 2045 | -1.955 -47.632 | 26.874 27.360 26.165 24.547 | 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 |
| MOTA MOTA | 13782 13783 13784 | NE CZ NH1 NH2 | ARG ARG ARG | 2045 2045 2045 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 | 26.874 27.360 26.165 24.547 25.031 | 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 |
| ATOM ATOM ATOM | 13782 13783 13784 13785 | NE CZ NH1 NH2 C | ARG ARG ARG ARG | 2045 2045 2045 2045 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 | 26.874 27.360 26.165 24.547 25.031 23.278 | 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 |
| ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 | NE CZ NH1 NH2 C | ARG ARG ARG ARG | 2045 2045 2045 2045 2045 2046 2046 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 | 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 |
| ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 | NE CZ NH1 NH2 C O N | ARG ARG ARG ARG ARG GLN | 2045 2045 2045 2045 2045 2046 2046 2046 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 | 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 |
| ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13789 13790 | NE CZ NH1 NH2 C O N CA CB | ARG ARG ARG ARG GLN GLN GLN GLN | 2045 2045 2045 2045 2045 2046 2046 2046 2046 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13789 13790 13791 | NE CZ NH1 NH2 C O C CA CB CG CD | ARG ARG ARG ARG GLN GLN GLN GLN GLN | 2045 2045 2045 2045 2046 2046 2046 2046 2046 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.737 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 21.49 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13789 13790 13791 13792 | NE CZ NH1 NH2 C O N CA CB CG CD OE1 | ARG ARG ARG ARG GLN GLN GLN GLN GLN GLN | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.737 18.687 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 21.49 24.59 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13789 13790 13791 13792 13793 | NE CZ NH1 NH2 C O N CA CB CG CD OE1 NE2 | ARG ARG ARG ARG GLN GLN GLN GLN GLN GLN GLN | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 | -1.955 -47.632 -2.874 -49.358 -3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.737 18.687 17.656 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 21.49 24.59 23.02 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13789 13790 13791 13792 13793 13794 | NE CZ NH1 NH2 C O N CA CB CG CD OE1 NE2 C | ARG ARG ARG ARG GLN GLN GLN GLN GLN GLN GLN GLN | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 2046 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.737 18.687 17.656 22.071 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 21.49 24.59 23.02 14.22 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13790 13791 13792 13793 13794 13795 | NE CZ NH1 NH2 C O N CA CB CG CD OE1 NE2 C | ARG ARG ARG ARG GLN GLN GLN GLN GLN GLN GLN GLN GLN GL | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 2046 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 6.624 -50.523 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.737 18.687 17.656 22.071 21.932 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 121.49 24.59 23.02 14.22 13.87 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13790 13791 13792 13793 13794 13795 13796 | NE CZ NH1 NH2 C O N CA CB CG CD OE1 NE2 C | ARG ARG ARG ARG GLN GLN GLN GLN GLN GLN GLN GLN GLN GL | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 2046 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 6.624 -50.523 5.821 -48.424 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.737 18.687 17.656 22.071 21.932 21.982 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 21.49 24.59 23.02 14.22 13.87 12.66 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13790 13791 13792 13793 13794 13795 13796 13797 | NE CZ NH1 NH2 C O N CA CB CG CD OE1 NE2 C O N CA | ARG ARG ARG ARG GLN GLN GLN GLN GLN GLN GLN GLN GLN GL | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 2046 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 6.624 -50.523 5.821 -48.424 7.136 -47.834 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.737 18.687 17.656 22.071 21.932 21.982 21.740 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 21.49 24.59 23.02 14.22 13.87 12.66 13.34 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13799 13799 13792 13793 13794 13795 13796 13797 13798 | NE CZ NH1 NH2 C O N CA CB CG CD OE1 NE2 C O N CA CB | ARG ARG ARG ARG GLN GLN GLN GLN GLN GLN GLN GLN GLN TYR TYR | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 2046 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 6.624 -50.523 5.821 -48.424 7.136 -47.834 6.993 -46.321 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.737 18.687 17.656 22.071 21.982 21.982 21.740 21.552 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 24.59 23.02 14.22 13.87 12.66 13.34 12.45 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13799 13791 13792 13793 13794 13795 13797 13798 13798 | NE CZ NH1 NH2 C O N CA CB CG CD OE1 NE2 C O N CA CB | ARG ARG ARG ARG GLN GLN GLN GLN GLN GLN TYR TYR TYR | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 2046 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 6.624 -50.523 5.821 -48.424 7.136 -47.834 6.993 -46.321 8.285 -45.548 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.737 17.656 22.071 21.982 21.982 21.740 21.552 21.643 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 21.49 24.59 23.02 14.22 13.87 12.66 13.34 12.45 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13790 13791 13792 13793 13794 13795 13796 13797 13797 13798 | NE CZ NH1 NH2 C O N CA CB CG CD OE1 NE2 C O N CA CB CG CD CA CB CG CD CA CB CG CD | ARG ARG ARG ARG GLN GLN GLN GLN GLN GLN TYR TYR TYR TYR | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 2046 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 6.624 -50.523 5.821 -48.424 7.136 -47.834 6.993 -46.321 8.285 -45.548 9.397 -45.883 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.737 17.656 22.071 21.932 21.740 21.552 21.643 20.855 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 21.49 24.59 23.02 14.22 13.87 12.66 13.34 12.45 13.33 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13790 13791 13792 13793 13794 13795 13796 13797 13798 13799 13800 13801 | NE CZ NH1 NH2 C O N CA CB CG OE1 NE2 C O N CA CB CC O CD CA CB CC CD CD | ARG ARG ARG ARG GLN GLN GLN GLN GLN GLN GLN TYR TYR TYR TYR TYR | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 2046 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 6.624 -50.523 5.821 -48.424 7.136 -47.834 6.993 -46.321 8.285 -45.548 9.397 -45.883 10.582 -45.148 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.737 18.687 17.656 22.071 21.932 21.740 21.552 21.643 20.855 20.940 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 21.49 24.59 23.02 14.22 13.87 12.66 13.34 12.45 13.33 12.66 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13790 13791 13792 13793 13794 13795 13796 13797 13798 13799 13800 13801 13802 | NE CZ NH1 NH2 C O N CA CB CG OE1 NE2 C O N CA CB CG CD CT CCA CB CG CD CT CCA CCB CCD CCD CCA CCB CCD CCD CCD CCD CCD CCD CCD CCD CCD | ARG ARG ARG ARG GLN GLN GLN GLN GLN GLN TYR TYR TYR TYR TYR TYR TYR | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 2046 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 6.624 -50.523 5.821 -48.424 7.136 -47.834 6.993 -46.321 8.285 -45.548 9.397 -45.883 10.582 -45.148 8.392 -44.469 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.737 17.656 22.071 21.932 21.982 21.740 21.552 21.643 20.855 20.940 22.510 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 21.49 24.59 23.02 14.22 13.87 12.66 13.34 12.45 13.33 12.65 13.34 12.45 13.35 12.65 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13790 13791 13792 13793 13795 13796 13797 13798 13799 13800 13801 13802 13803 | NE CZ NH1 NH2 C O N CA CB CG OE1 NE2 C O N CA CB CG CD CCA CCB CCB CCC CCB CCC CCC CCC CCC CCC | ARG ARG ARG ARG GLN GLN GLN GLN GLN GLN GLN TYR TYR TYR TYR TYR TYR TYR TYR | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 2047 2047 2047 2047 2047 2047 2047 2047 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 6.624 -50.523 5.821 -48.424 7.136 -47.834 6.993 -46.321 8.285 -45.548 9.397 -45.883 10.582 -45.148 8.392 -44.469 9.557 -43.735 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.687 17.656 22.071 21.932 21.940 21.552 21.643 20.855 20.940 22.510 22.601 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 24.59 23.02 14.22 13.87 12.66 13.34 12.45 13.33 12.66 15.89 15.90 14.07 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13799 13792 13793 13794 13795 13796 13797 13798 13799 13800 13801 13801 13803 13804 | NE CZ NH1 NH2 C O N CA CB CG CD OE1 NE2 C O N CA CB CG CD1 CCA CCB CCC CCD CCA CCB CCC CCC CCC CCC CCC CCC | ARG ARG ARG ARG GLN GLN GLN GLN GLN GLN TYR TYR TYR TYR TYR TYR TYR TYR | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 2047 2047 2047 2047 2047 2047 2047 2047 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 6.624 -50.523 5.821 -48.424 7.136 -47.834 6.993 -46.321 8.285 -45.548 9.397 -45.883 10.582 -45.148 8.392 -44.469 9.557 -43.735 10.649 -44.068 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 21.982 21.982 21.740 21.552 21.643 20.855 20.940 22.510 22.510 22.510 21.824 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 24.59 23.02 14.22 13.87 12.66 13.34 12.45 13.33 12.66 15.05 17.14 18.07 19 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13790 13791 13792 13793 13794 13795 13798 13799 13800 13801 13802 13804 13805 | NE CZ NH1 NH2 C O N CA CB CG CD OE1 NE2 C O CA CB CG CD CCA CCB CCB CCD CCB CCB CCB CCD CCB CCB CCB | ARG ARG ARG ARG GLN GLN GLN GLN GLN GLN TYR | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 2047 2047 2047 2047 2047 2047 2047 2047 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 6.624 -50.523 5.821 -48.424 7.136 -47.834 6.993 -46.321 8.285 -45.548 9.397 -45.883 10.582 -45.148 8.392 -44.469 9.557 -43.735 10.649 -44.068 11.805 -43.318 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.737 17.656 22.071 21.982 21.740 21.552 21.643 20.855 20.940 22.510 22.601 21.824 21.929 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 21.49 24.59 23.02 14.22 13.87 12.66 13.34 12.45 13.33 12.66 13.34 14.07 14.07 14.07 14.09 16.90 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13790 13791 13792 13793 13794 13795 13796 13797 13799 13800 13801 13802 13803 13804 13805 13806 | NE CZ NH1 NH2 C O N CA CB CG CD OE1 CE1 CD2 CE2 CD CDC CD CDC CD CDC CD CDC CDC CDC CC C | ARG ARG ARG ARG GLN GLN GLN GLN GLN TYR | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 2047 2047 2047 2047 2047 2047 2047 2047 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 6.624 -50.523 5.821 -48.424 7.136 -47.834 6.993 -46.321 8.285 -45.548 9.397 -45.883 10.582 -45.148 8.392 -44.469 9.557 -43.735 10.649 -44.068 11.805 -43.318 8.030 -48.163 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.737 17.656 22.071 21.932 21.740 21.552 21.643 20.855 20.940 22.510 22.601 21.929 22.939 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 13.65 17.14 21.49 24.59 23.02 14.22 13.87 12.66 13.34 12.45 13.33 12.66 14.07 14.07 14.99 14.99 12.59 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13789 13790 13791 13792 13793 13796 13797 13798 13799 13800 13801 13802 13803 13804 13805 13806 13807 | NE CZ NH1 NH2 C O N CA CB CG OE1 NE2 C O N CA CB CCD OE1 CD2 CCA CB CCB CCD CD1 CD2 CCD CCD | ARG ARG ARG ARG GLN GLN GLN GLN GLN TYR | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 2047 2047 2047 2047 2047 2047 2047 2047 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 6.624 -50.523 5.821 -48.424 7.136 -47.834 6.993 -46.321 8.285 -45.548 9.397 -45.883 10.582 -45.148 8.392 -44.469 9.557 -43.735 10.649 -44.068 11.805 -43.318 8.030 -48.163 9.145 -48.661 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.737 18.687 17.656 22.071 21.932 21.740 21.552 21.643 20.855 20.940 22.510 22.601 21.824 21.929 22.939 22.784 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 21.49 24.59 23.02 14.22 13.87 12.66 13.34 12.45 13.33 12.66 15.89 12.07 14.07 14.07 14.94 16.90 12.59 10.64 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13790 13791 13792 13793 13794 13795 13796 13797 13798 13799 13800 13801 13802 13803 13804 13805 13806 13807 13808 | NE CZ NH1 NH2 C O N CA CB CCD OE1 NE2 C O N CA CB CCB CCD CCA CCB CCD CCD N | ARG ARG ARG ARG ARG GLN GLN GLN GLN GLN TYR | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 2047 2047 2047 2047 2047 2047 2047 2047 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 6.624 -50.523 5.821 -48.424 7.136 -47.834 6.993 -46.321 8.285 -45.548 9.397 -45.883 10.582 -45.148 8.392 -44.469 9.557 -43.735 10.649 -44.068 11.805 -43.318 8.030 -48.163 9.145 -48.661 7.522 -47.896 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.687 17.656 22.071 21.932 21.740 21.552 21.643 20.855 20.940 22.510 22.601 21.824 21.929 22.939 22.784 24.139 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 21.49 24.59 23.02 14.22 13.87 12.66 13.34 12.45 13.33 12.66 15.89 12.07 14.94 16.90 12.59 10.64 12.77 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13799 13792 13793 13794 13795 13797 13798 13799 13800 13801 13802 13803 13804 13805 13806 13808 13808 | NE CZ NH1 NH2 C O N CA CB CG CD OE1 CE2 CZ OH C CZ OH CA CE2 CZ OH CA CA | ARG ARG ARG ARG GLN GLN GLN GLN GLN GLN TYR | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2047 2047 2047 2047 2047 2047 2047 2047 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 6.624 -50.523 5.821 -48.424 7.136 -47.834 6.993 -46.321 8.285 -45.548 9.397 -45.883 10.582 -45.148 8.392 -44.469 9.557 -43.735 10.649 -44.068 11.805 -43.318 8.030 -48.163 9.145 -48.661 7.522 -47.896 8.266 -48.190 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.687 17.656 22.071 21.982 21.982 21.740 21.552 21.643 20.855 20.940 22.601 21.824 21.929 22.939 22.784 24.139 25.361 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 24.59 23.02 14.22 13.87 12.66 13.34 12.45 13.33 12.66 15.89 14.07 14.94 16.90 12.59 12.59 13.61 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 13782 13783 13784 13785 13786 13787 13788 13790 13791 13792 13793 13794 13795 13796 13797 13798 13799 13800 13801 13802 13803 13804 13805 13806 13807 13808 | NE CZ NH1 NH2 C O N CA CB CCD OE1 NE2 C O N CA CB CCB CCD CCA CCB CCD CCD N | ARG ARG ARG ARG ARG GLN GLN GLN GLN GLN TYR | 2045 2045 2045 2045 2046 2046 2046 2046 2046 2046 2046 2047 2047 2047 2047 2047 2047 2047 2047 | -1.955 -47.632 -2.874 -49.358 3.986 -49.265 4.925 -49.897 3.604 -49.373 4.279 -50.255 3.503 -50.340 4.052 -51.389 3.320 -51.419 2.098 -51.286 4.063 -51.607 5.682 -49.742 6.624 -50.523 5.821 -48.424 7.136 -47.834 6.993 -46.321 8.285 -45.548 9.397 -45.883 10.582 -45.148 8.392 -44.469 9.557 -43.735 10.649 -44.068 11.805 -43.318 8.030 -48.163 9.145 -48.661 7.522 -47.896 | 26.874 27.360 26.165 24.547 25.031 23.278 22.343 21.027 20.066 18.687 17.656 22.071 21.932 21.740 21.552 21.643 20.855 20.940 22.510 22.601 21.824 21.929 22.939 22.784 24.139 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 19.90 18.74 17.78 11.67 13.65 11.60 13.89 15.05 17.14 21.49 24.59 23.02 14.22 13.87 12.66 13.34 12.45 13.33 12.66 15.89 12.07 14.94 16.90 12.59 10.64 12.77 |

| MOTA | 13812 | SD | MET | 2048 | | 5.856 | -46.160 | 28.106 | 1.00 | 18.28 |
|------|-------|------|-----|------|---|--------|---------|--------|------|-------|
| ATOM | 13813 | CE | MET | 2048 | | 6.752 | -46.711 | 29.577 | 1.00 | 18.21 |
| ATOM | 13814 | C | MET | 2048 | | | -49.647 | 25.400 | 1.00 | 14.55 |
| | | | | 2048 | | | -49.941 | 25.652 | 1.00 | 11.07 |
| MOTA | 13815 | 0 | MET | | | | | | | |
| MOTA | 13816 | N | ALA | 2049 | | | -50.561 | 25.163 | 1.00 | 13.04 |
| MOTA | 13817 | CA | ALA | 2049 | | | -51.988 | 25.182 | 1.00 | 14.89 |
| MOTA | 13818 | CB | ALA | 2049 | | 6.798 | -52.799 | 24.992 | 1.00 | 14.38 |
| MOTA | 13819 | С | ALA | 2049 | | 9.128 | -52.385 | 24.130 | 1.00 | 15.06 |
| ATOM | 13820 | O | ALA | 2049 | | 10.043 | -53.163 | 24.414 | 1.00 | 14.34 |
| ATOM | 13821 | N | GLU | 2050 | | | -51.849 | 22.916 | 1.00 | 12.60 |
| | | | | 2050 | | | -52.224 | 21.869 | | 13.77 |
| MOTA | 13822 | CA | GLU | | | | | | | |
| MOTA | 13823 | CB | GLU | 2050 | | | -51.778 | 20.480 | 1.00 | 10.52 |
| MOTA | 13824 | CG | GLU | 2050 | | | -52.697 | 19.915 | 1.00 | 12.90 |
| MOTA | 13825 | CD - | GLU | 2050 | | 7.895 | -52.284 | 18.544 | 1.00 | 14.19 |
| ATOM | 13826 | OE1 | GLU | 2050 | | 8.707 | -51.760 | 17.752 | 1.00 | 14.22 |
| ATOM | 13827 | OE2 | GLU | 2050 | | 6.695 | -52.502 | 18.255 | 1.00 | 13.57 |
| ATOM | 13828 | С | GLU | 2050 | | 11.361 | -51.689 | 22.145 | 1.00 | 14.61 |
| ATOM | 13829 | ō | GLU | 2050 | | | -52.322 | 21.790 | 1.00 | 12.04 |
| | | N | VAL | 2051 | | | -50.528 | 22.783 | 1.00 | 14.04 |
| MOTA | 13830 | | | | | | | | | 12.24 |
| MOTA | 13831 | CA | VAL | 2051 | | | -49.999 | 23.088 | 1.00 | |
| MOTA | 13832 | CB | VAL | 2051 | | | -48.552 | 23.589 | | 12.65 |
| MOTA | 13833 | CG1 | VAL | 2051 | | | -48.153 | 24.216 | 1.00 | 12.32 |
| MOTA | 13834 | CG2 | VAL | 2051 | | 12.361 | -47.621 | 22.427 | 1.00 | 10.30 |
| ATOM | 13835 | С | VAL | 2051 | | 13.434 | -50.866 | 24.159 | 1.00 | 12.70 |
| ATOM | 13836 | 0 | VAL | 2051 | | 14.618 | -51.203 | 24.063 | 1.00 | 14.76 |
| ATOM | 13837 | N | GLU | 2052 | | | -51.232 | 25.177 | 1.00 | 12.67 |
| ATOM | 13838 | | GLU | 2052 | | | -52.051 | 26.267 | 1.00 | 13.06 |
| | | CA | | | | | | | | 17.19 |
| ATOM | 13839 | СВ | GLU | 2052 | | | -52.152 | 27.405 | | |
| MOTA | 13840 | CG | GLU | 2052 | | | -52.976 | 28.597 | 1.00 | 22.09 |
| MOTA | 13841 | CD | GLU | 2052 | | 11.791 | -52.760 | 29.836 | 1.00 | 27.02 |
| ATOM | 13842 | OE1 | GLU | 2052 | | 11.779 | -53.647 | 30.714 | 1.00 | 29.74 |
| MOTA | 13843 | OE2 | GLU | 2052 | | 11.135 | -51.702 | 29.940 | 1.00 | 27.52 |
| ATOM | 13844 | С | GLU | 2052 | | | -53.446 | 25.809 | 1.00 | 15.04 |
| ATOM | 13845 | ō | GLU | 2052 | | | -54.006 | 26.299 | | 12.91 |
| | 13846 | N | SER | 2053 | | | -54.005 | 24.862 | | 14.34 |
| ATOM | | | | | | | | | | |
| ATOM | 13847 | CA | SER | 2053 | | | -55.336 | 24.349 | 1.00 | 16.44 |
| MOTA | 13848 | CB | SER | 2053 | | | -55.945 | 23.689 | 1.00 | 17.92 |
| ATOM | 13849 | OG | SER | 2053 | | | -56.242 | 24.665 | 1.00 | 29.42 |
| MOTA | 13850 | С | SER | 2053 | | 14.306 | -55.292 | 23.337 | 1.00 | 16.59 |
| MOTA | 13851 | 0 | SER | 2053 | | 14.868 | -56.326 | 22.994 | 1.00 | 16.54 |
| MOTA | 13852 | N | GLY | 2054 | | 14.632 | -54.096 | 22.856 | 1.00 | 14.35 |
| ATOM | 13853 | CA | GLY | 2054 | | 15.695 | -53.961 | 21.877 | 1.00 | 14.92 |
| ATOM | 13854 | C | GLY | 2054 | | | -54.137 | 20.464 | 1.00 | 14.49 |
| | | | | | | | -54.058 | 19.503 | 1.00 | 14.84 |
| ATOM | 13855 | 0 | GLY | 2054 | | | | | | |
| MOTA | 13856 | N | VAL | 2055 | | | -54.379 | 20.347 | | 13.75 |
| MOTA | 13857 | CA | VAL | 2055 | | | -54.582 | 19.061 | | 16.33 |
| MOTA | 13858 | CB | VAL | 2055 | | | -55.006 | 19.312 | | 19.13 |
| ATOM | 13859 | CG1 | VAL | 2055 | | 10.824 | -54.610 | 18.157 | 1.00 | 24.52 |
| ATOM | 13860 | CG2 | VAL | 2055 | | 11.640 | -56.508 | 19.561 | 1.00 | 22.18 |
| ATOM | 13861 | С | VAL | 2055 | | 13.203 | -53.333 | 18.181 | 1.00 | 15.78 |
| ATOM | 13862 | 0 - | VAL | 2055 | | | -53.420 | 16.953 | | 14.79 |
| ATOM | 13863 | N | TYR | 2056 | | | -52.177 | 18.823 | | 13.64 |
| | | | | | | | -50.895 | 18.121 | | 14.23 |
| ATOM | 13864 | CA | TYR | 2056 | | | | | | |
| MOTA | 13865 | CB | TYR | 2056 | | | -50.108 | 18.336 | 1.00 | 14.11 |
| MOTA | 13866 | CG | TYR | 2056 | | | -48.760 | 17.647 | 1.00 | 13.46 |
| ATOM | 13867 | CD1 | TYR | 2056 | | | -48.653 | 16.270 | 1.00 | 14.58 |
| MOTA | 13868 | CE1 | TYR | 2056 | | 11.857 | -47.443 | 15.605 | | 13.65 |
| ATOM | 13869 | CD2 | TYR | 2056 | | 12.248 | -47.614 | 18.349 | 1.00 | 11.87 |
| ATOM | 13870 | CE2 | TYR | 2056 | | | -46.397 | 17.696 | | 13.86 |
| ATOM | 13871 | CZ | TYR | 2056 | | | -46.323 | 16.326 | | 14.29 |
| ATOM | 13871 | ОН | TYR | 2056 | | | -45.134 | 15.671 | | 14.14 |
| | | | | | | | | | | |
| MOTA | 13873 | C | TYR | 2056 | | | -50.086 | 18.691 | | 13.20 |
| MOTA | 13874 | 0 | TYR | 2056 | | | -49.991 | 19.901 | | 13.24 |
| MOTA | 13875 | N | PRO | 2057 | | | -49.477 | 17.825 | | 15.12 |
| MOTA | 13876 | CD | PRO | 2057 | • | | -48.516 | 18.218 | 1.00 | 16.15 |
| ATOM | 13877 | CA | PRO | 2057 | | 14.952 | -49.547 | 16.371 | 1.00 | 15.54 |
| ATOM | 13878 | CB | PRO | 2057 | | 15.799 | -48.374 | 15.880 | 1.00 | 18.49 |
| MOTA | 13879 | CG | PRO | 2057 | | | -48.270 | 16.917 | 1.00 | 17.17 |
| ATOM | 13880 | C | PRO | 2057 | | | -50.876 | 15.763 | 1.00 | 17.76 |
| | | | | | | | -51.580 | | 1.00 | 16.91 |
| MOTA | 13881 | 0 | PRO | 2057 | | | | | | |
| MOTA | 13882 | N | GLY | 2058 | | | -51.223 | 14.646 | 1.00 | 16.96 |
| ATOM | 13883 | CA | GLY | 2058 | | | -52.457 | 13.951 | 1.00 | 18.25 |
| MOTA | 13884 | С | GLY | 2058 | | | -52.181 | 12.932 | 1.00 | 19.23 |
| MOTA | 13885 | 0 | GLY | 2058 | | | -51.039 | 12.776 | | 17.91 |
| MOTA | 13886 | N | GLU | 2059 | | 16.590 | -53.220 | 12.234 | | 18.48 |
| ATOM | 13887 | CA | GLU | 2059 | | 17.627 | -53.048 | 11.225 | 1.00 | 19.82 |
| | | | | | | | -54.396 | 10.572 | 1.00 | 22.37 |
| ATOM | 13888 | CB | GLU | 2059 | | | | | | |

| ATOM | 13889 | CG | GLU | 2059 | 19.024 | -54.287 | 9.491 | 1.00 25.19 |
|--------------------------------------|--|--------------------------|---------------------------------|------------------------------|--|--|--|--|
| | 13890 | CD | GLU | 2059 | | -53.864 | 10.050 | 1.00 26.27 |
| ATOM | | | | | | | | |
| MOTA | 13891 | OE1 | | 2059 | | -53.288 | 9.285 | 1.00 28.76 |
| ATOM | 13892 | OE2 | GLU | 2059 | 20.637 | -54.117 | 11.246 | 1.00 24.77 |
| ATOM | 13893 | C | GLU | 2059 | 17.193 | -52.054 | 10.151 | 1.00 17.71 |
| ATOM | 13894 | 0 | GLU | 2059 | 18 007 | -51.273 | 9.657 | 1.00 16.86 |
| | | | | | | | | |
| MOTA | 13895 | N | GLU | 2060 | | -52.078 | 9.797 | 1.00 18.39 |
| MOTA | 13896 | CA | GLU | 2060 | 15.388 | -51.179 | 8.764 | 1.00 19.58 |
| ATOM | 13897 | CB | GLU | 2060 | 13.936 | -51.506 | 8.433 | 1.00 23.58 |
| | 13898 | CG | GLU | 2060 | | -52.954 | 8.501 | 1.00 29.46 |
| MOTA | | | | | | | | |
| ATOM | 13899 | CD | GLU | 2060 | | -53.188 | 9.527 | 1.00 30.54 |
| MOTA | 13900 | . OE1 | GLU | 2060 | 11.392 | -52.590 | 9.370 | 1.00 31.23 |
| MOTA | 13901 | OE2 | GLU | 2060 | 12.724 | -53.954 | 10.484 | 1.00 34.44 |
| ATOM | 13902 | С | GLU | 2060 | 15.443 | -49.723 | 9.197 | 1.00 18.24 |
| | | | | | | -48.828 | 8.363 | 1.00 18.32 |
| MOTA | 13903 | 0 | GLU | 2060 | | | | |
| ATOM | 13904 | N | HIS | 2061 | 15.592 | -49.495 | 10.499 | 1.00 17.85 |
| MOTA | 13905 | CA | HIS | 2061 | 15.646 | -48.138 | 11.050 | 1.00 15.77 |
| ATOM | 13906 | CB | HIS | 2061 | 14.890 | -48.075 | 12.374 | 1.00 15.70 |
| ATOM | 13907 | CG | HIS | 2061 | | -48.573 | 12.296 | 1.00 13.96 |
| | | | | | | | | |
| ATOM | 13908 | | HIS | 2061 | | -49.609 | 12.912 | 1.00 11.61 |
| ATOM | 13909 | ND1 | HIS | 2061 | 12.526 | -47.964 | 11.518 | 1.00 14.67 |
| ATOM | 13910 | CE1 | HIS | 2061 | 11.378 | -48.601 | 11.660 | 1.00 12.03 |
| ATOM | 13911 | NE2 | HIS | 2061 | 11.559 | ~49.603 | 12.500 | 1.00 17.48 |
| | | | | | | | 11.324 | 1.00 16.96 |
| MOTA | 13912 | C | HIS | 2061 | | -47.702 | | |
| ATOM | 13913 | 0 | HIS | 2061 | | -46.639 | 11.899 | 1.00 16.77 |
| ATOM | 13914 | N | SER | 2062 | 18.040 | -48.516 | 10.913 | 1.00 17.85 |
| ATOM | 13915 | CA | SER | 2062 | 19.449 | -48.230 | 11.175 | 1.00 18.95 |
| MOTA | 13916 | CB | SER | 2062 | | -49.420 | 11.926 | 1.00 18.81 |
| | | | | | | | | |
| MOTA | 13917 | OG | SER | 2062 | | -49.760 | 13.059 | 1.00 21.12 |
| ATOM | 13918 | C | SER | 2062 | 20.298 | -47.917 | 9.941 | 1.00 21.62 |
| ATOM | 13919 | 0 | SER | 2062 | 19.945 | -48.283 | 8.813 | 1.00 21.18 |
| ATOM | 13920 | N | PHE | 2063 | | -47.240 | 10.170 | 1.00 22.99 |
| | | | | | | | 9.099 | 1.00 26.28 |
| MOTA | 13921 | CA | PHE | 2063 | | -46.870 | | |
| MOTA | 13922 | CB | PHE | 2063 | 22.600 | -45.348 | 9.075 | 1.00 26.42 |
| ATOM | 13923 | CG | PHE | 2063 | 21.360 | -44.526 | 8.820 | 1.00 29.55 |
| ATOM | 13924 | CD1 | PHE | 2063 | 20.806 | -43.746 | 9.835 | 1.00 31.06 |
| | 13925 | | PHE | 2063 | | -44.519 | 7.568 | 1.00 29.76 |
| MOTA | | | | | | | | |
| MOTA | 13926 | | PHE | 2063 | | -42.974 | 9.607 | 1.00 30.50 |
| MOTA | 13927 | CE2 | PHE | 2063 | 19.610 | -43.750 | 7.328 | 1.00 31.05 |
| ATOM | 13928 | CZ | PHE | 2063 | 19.065 | -42.976 | 8.350 | 1.00 29.87 |
| ATOM | 13929 | C | PHE | 2063 | | -47.577 | 9.301 | 1.00 26.42 |
| | | | | | | | | |
| ATOM | 13930 | 0 | PHE | 2063 | | -47.849 | 10.432 | 1.00 22.96 |
| ATOM | 13931 | N | HIS | 2064 | 24.386 | -47.867 | 8.199 | 1.00 28.64 |
| MOTA | 13932 | CA | HIS | 2064 | 25.687 | -48.543 | 8.246 | 1.00 31.07 |
| ATOM | 13933 | СВ | HIS | 2064 | | -49.996 | 7.789 | 1.00 31.23 |
| | | | | | | -50.855 | 8.749 | 1.00 31.06 |
| MOTA | 13934 | CG | HIS | 2064 | | | | |
| ATOM | 13935 | | HIS | 2064 | | -51.345 | 8.704 | 1.00 30.91 |
| MOTA | 13936 | ND1 | HIS | 2064 | 25.320 | -51.287 | 9.943 | 1.00 32.43 |
| ATOM | 13937 | CE1 | HIS | 2064 | 24.423 | -52.007 | 10.593 | 1.00 32.22 |
| ATOM | 13938 | NE2 | HIS | 2064 | | -52.058 | 9.863 | 1.00 32.35 |
| | | | | | | | | 1.00 31.64 |
| MOTA | 13939 | С | HIS | 2064 | | -47.836 | 7.381 | |
| ATOM | 13940 | 0 | HIS | 2064 | | -47.757 | 7.818 | 1.00 32.53 |
| MOTA | 13941 | OXT | HIS | 2064 | 26.375 | -47.385 | 6.272 | 1.00 34.83 |
| ATOM | 13942 | C1 | KPL | 2065 | 15.474 | -35.267 | 17.263 | 1.00 36.48 |
| ATOM | 13943 | C2 | KPL | 2065 | | -34.899 | 18.622 | 1.00 35.77 |
| | | | | | | | | |
| MOTA | 13944 | C3 | KPL | 2065 | | -35.486 | 19.739 | |
| MOTA | 13945 | C4 | KPL | 2065 | | -35.515 | 18.719 | 1.00 37.71 |
| ATOM | 13946 | 01 | KPL | 2065 | 18.376 | -35.011 | 17.682 | 1.00 42.74 |
| ATOM | 13947 | C5 | KPL | 2065 | 16.164 | -33.356 | 18.773 | 1.00 32.73 |
| ATOM | 13948 | 02 | KPL | 2065 | | -32.800 | 18.938 | 1.00 31.75 |
| | | | | | | | | |
| MOTA | 13949 | C6 | KPL | 2065 | | -32.498 | 18.721 | 1.00 31.70 |
| MOTA | 13950 | 03 | KPL | 2065 | 13.821 | -33.000 | 18.568 | 1.00 31.03 |
| MOTA | 13951 | 04 | KPL | 2065 | 15.041 | -31.157 | 18.845 | 1.00 20.56 |
| ATOM | 13952 | CB | MET | 2101 | 22.414 | -8.383 | 70.247 | 1.00 66.53 |
| MOTA | 13953 | CG | MET | 2101 | 22.617 | -8.021 | 71.717 | 1.00 69.29 |
| | | | | | | | | |
| MOTA | 13954 | SD | MET | 2101 | 22.027 | -6.373 | 72.186 | 1.00 72.42 |
| MOTA | 13955 | CE | MET | 2101 | 23.584 | -5.466 | 72.275 | 1.00 72.02 |
| MOTA | 13956 | С | MET | 2101 | 22.338 | -6.232 | 68.953 | 1.00 62.58 |
| | | Ō | MET | 2101 | 21.157 | -6.314 | 68.610 | 1.00 62.34 |
| WI Chai | 13957 | | MET | | 24.527 | -7.178 | 69.751 | 1.00 64.37 |
| ATOM | 13957 | | | 2101 | | | | |
| ATOM | 13958 | N | | | | | | 1 00 64 20 |
| MOTA MOTA | 13958 13959 | N CA | MET | 2101 | 23.158 | -7.490 | 69.244 | 1.00 64.28 |
| ATOM | 13958 | N | | 2101 2102 | 23.158 | -5.073 | 69.085 | 1.00 60.08 |
| ATOM ATOM ATOM | 13958 13959 13960 | N CA N | MET LYS | 2102 | | | | |
| MOTA MOTA MOTA MOTA | 13958 13959 13960 13961 | N CA N CA | MET LYS LYS | 2102 2102 | 22.975 22.317 | -5.073 -3.798 | 69.085 68.834 | 1.00 60.08 1.00 57.36 |
| ATOM ATOM ATOM ATOM ATOM | 13958 13959 13960 13961 13962 | N CA N CA CB | MET LYS LYS LYS | 2102 2102 2102 | 22.975 22.317 22.010 | -5.073 -3.798 -3.086 | 69.085 68.834 70.157 | 1.00 60.08 1.00 57.36 1.00 58.35 |
| ATOM ATOM ATOM ATOM ATOM | 13958 13959 13960 13961 13962 13963 | N CA N CA CB | MET LYS LYS LYS LYS | 2102 2102 2102 2102 | 22.975 22.317 22.010 20.762 | -5.073 -3.798 -3.086 -3.591 | 69.085 68.834 70.157 70.868 | 1.00 60.08 1.00 57.36 1.00 58.35 1.00 60.33 |
| ATOM ATOM ATOM ATOM ATOM | 13958 13959 13960 13961 13962 | N CA N CA CB | MET LYS LYS LYS | 2102 2102 2102 | 22.975 22.317 22.010 20.762 19.496 | -5.073 -3.798 -3.086 -3.591 -3.202 | 69.085 68.834 70.157 70.868 70.117 | 1.00 60.08 1.00 57.36 1.00 58.35 1.00 60.33 1.00 61.31 |
| ATOM ATOM ATOM ATOM ATOM | 13958 13959 13960 13961 13962 13963 | N CA N CA CB | MET LYS LYS LYS LYS | 2102 2102 2102 2102 | 22.975 22.317 22.010 20.762 | -5.073 -3.798 -3.086 -3.591 | 69.085 68.834 70.157 70.868 | 1.00 60.08 1.00 57.36 1.00 58.35 1.00 60.33 |

| MOTA | 13966 | NZ | LYS | 2102 | 18.073 | -1.296 | 69.354 | 1.00 | 63.75 |
|--------------|----------------|------------|------------|--------------|------------------|--------------------|------------------|------|----------------|
| ATOM | 13967 | С | LYS | 2102 | 23.179 | -2.896 | 67.957 | | 54.18 |
| ATOM | 13968 | 0 | LYS | 2102 | 23.678 | -1.865 | 68.413 | | 54.59 |
| ATOM | 13969 | N | PRO | 2103 | 23.371 | -3.276 | 66.685 | | 50.17 |
| ATOM | 13970 | CD | PRO PRO | 2103 2103 | 23.878 22.830 | -2.346 -4.484 | 65.660 66.053 | | 49.96 46.64 |
| MOTA MOTA | 13971 13972 | CA CB | PRO | 2103 | 22.605 | -4.464 | 64.620 | | 47.38 |
| ATOM | 13973 | CG | PRO | 2103 | 23.802 | -3.176 | 64.386 | | 48.98 |
| ATOM | 13974 | C | PRO | 2103 | 23.794 | -5.673 | 66.131 | | 42.70 |
| MOTA | 13975 | 0 | PRO | 2103 | 24.924 | -5.536 | 66.596 | 1.00 | 41.32 |
| MOTA | 13976 | N | THR | 2104 | 23.334 | -6.832 · | | | 38.31 |
| MOTA | 13977 | CA | THR | 2104 | 24.144 | -8.045 | 65.662 | | 35.00 |
| ATOM | 13978 13979 | CB OC1 | THR | 2104 | 23.259 | -9.309 -9.286 | 65.701 66.875 | | 35.04 34.66 |
| ATOM ATOM | 13979 | OG1 CG2 | THR THR | 2104 2104 | 22.442 24.116 | -10.561 | 65.714 | | 34.54 |
| ATOM | 13981 | C | THR | 2104 | 24.981 | -8.080 | 64.384 | | 33.55 |
| ATOM | 13982 | 0 | THR | 2104 | 24.455 | -7.872 | 63.291 | | 31.34 |
| MOTA | 13983 | N | THR | 2105 | 26.279 | -8.340 | 64.521 | | 31.77 |
| MOTA | 13984 | CA | THR | 2105 | 27.172 | -8.391 | 63.365 | | 30.32 |
| ATOM | 13985 | CB | THR | 2105 | 28.127 | -7.175 | 63.336 | | 30.72 |
| ATOM ATOM | 13986 13987 | OG1 CG2 | THR THR | 2105 2105 | 28.999 27.338 | -7.223 -5.874 | 64.471 63.366 | | 32.36 29.57 |
| ATOM | 13988 | CGZ | THR | 2105 | 28.013 | -9.664 | 63.355 | | 29.36 |
| ATOM | 13989 | ō | THR | 2105 | | -10.474 | 64.281 | | 29.05 |
| ATOM | 13990 | N | ILE | 2106 | 28.798 | -9.837 | 62.297 | 1.00 | 28.45 |
| ATOM | 13991 | CA | ILE | 2106 | 29.666 | -11.004 | 62.162 | 1.00 | 28.68 |
| MOTA | 13992 | CB | ILE | 2106 | | -10.912 | 60.893 | | 28.87 |
| MOTA | 13993 | CG2 | ILE | 2106 | | -12.221 | 60.690 | | 28.27 |
| ATOM | 13994 | CG1 | ILE | 2106 | 29.639 | -10.618 -10.317 | 59.681 | | 31.64 |
| ATOM | 13995 13996 | CD1 C | ILE ILE | 2106 2106 | | -10.317 | 58.403 63.364 | | 31.18 29.36 |
| MOTA MOTA | 13997 | 0 | ILE | 2106 | | -12.164 | 63.833 | | 29.25 |
| ATOM | 13998 | N | SER | 2107 | 31.003 | -9.912 | 63.854 | | 29.55 |
| ATOM | 13999 | CA | SER | 2107 | 31.897 | -9.820 | 65.002 | 1.00 | 30.81 |
| MOTA | 14000 | CB · | SER | 2107 | 32.058 | -8.358 | 65.425 | | 31.74 |
| MOTA | 14001 | OG | SER | 2107 | 32.548 | -7.568 | 64.361 | | 34.72 |
| ATOM | 14002 | С | SER | 2107 | | -10.632 | 66.175 | | 29.75 |
| MOTA | 14003 | 0 | SER | 2107 | 32.131 | -11.245 | 66.904 66.348 | | 29.24 29.42 |
| ATOM ATOM | 14004 14005 | N CA | LEU LEU | 2108 2108 | | -10.630 -11.368 | 67.436 | | 29.77 |
| MOTA | 14006 | CB | LEU | 2108 | 27.925 | -11.045 | 67.512 | | 30.86 |
| ATOM | 14007 | CG | LEU | 2108 | | -10.598 | 68.865 | | 32.78 |
| MOTA | 14008 | CD1 | LEU | 2108 | 25.830 | -10.637 | 68.802 | 1.00 | 33.38 |
| MOTA | 14009 | | LEU | 2108 | | -11.506 | 69.983 | | 32.44 |
| ATOM | 14010 | C · | | 2108 | 29.601 | -12.874 | 67.267 | | 29.98 |
| ATOM | 14011 | 0 | LEU LEU | 2108 2109 | 29.949 29.366 | -13.575 -13.369 | 68.216 66.055 | | 28.71 28.45 |
| ATOM ATOM | 14012 14013 | N CA | LEU | 2109 | 29.504 | -14.795 | 65.783 | | 28.96 |
| ATOM | 14014 | СВ | LEU | 2109 | | -15.112 | 64.360 | | 26.96 |
| АТОМ | 14015 | CG | LEU | 2109 | | -14.653 | 63.997 | | 26.16 |
| MOTA | 14016 | CD1 | LEU | 2109 | 27.228 | -15.201 | 62.628 | 1.00 | 24.61 |
| MOTA | 14017 | | LEU | 2109 | | -15.140 | 65.046 | | 23.92 |
| ATOM | 14018 | C | LEU | 2109 | | -15.232 | 65.962 | | 30.20 |
| ATOM ATOM | 14019 14020 | O N | LEU GLN | 2109 2110 | 31.234 | -16.329 -14.366 | 66.455 65.563 | | 27.70 32.67 |
| ATOM | 14020 | N CA | GLN | 2110 | | -14.666 | 65.691 | | 35.69 |
| ATOM | 14022 | СВ | GLN | 2110 | 34.131 | -13.556 | 65.041 | | 37.71 |
| ATOM | 14023 | CG | GLN | 2110 | | -13.909 | 64.805 | | 40.40 |
| ATOM | 14024 | CD | GLN | 2110 | | -15.115 | 63.894 | | 41.71 |
| MOTA | 14025 | OE1 | GLN | 2110 | | -16.259 | 64.303 | | 42.12 |
| MOTA | 14026 | NE2 | | 2110 | | -14.858 | 62.645 | | 42.57 |
| MOTA | 14027 | C | GLN | 2110 | | -14.778 -15.595 | 67.179 67.588 | | 37.51 39.31 |
| ATOM ATOM | 14028 14029 | O N | GLN LYS | 2110 2111 | | -13.956 | 67.987 | | 38.46 |
| ATOM | 14030 | CA | LYS | 2111 | | -13.980 | 69.430 | | 39.03 |
| ATOM | 14031 | СВ | LYS | 2111 | | -12.824 | 70.098 | | 41.13 |
| MOTA | 14032 | CG | LYS | 2111 | | -12.839 | 71.621 | | 44.09 |
| MOTA | 14033 | CD | LYS | 2111 | | -12.035 | 72.275 | | 45.16 |
| ATOM | 14034 | CE | LYS | 2111 | | -10.557 | 71.933 | | 46.74 |
| MOTA | 14035 | NZ | LYS | 2111 | 30.408 | -9.785 -15.301 | 72.674 | | 47.25 38.63 |
| ATOM ATOM | 14036 14037 | C 0 | LYS LYS | 2111 2111 | 32.637 | -15.301 -15.931 | 69.989 70.825 | | 37.38 |
| ATOM | 14037 | N | TYR | 2111 | | -15.714 | 69.521 | | 38.15 |
| ATOM | 14039 | CA | TYR | 2112 | | -16.959 | 69.970 | | 37.96 |
| ATOM | 14040 | СВ | TYR | 2112 | | -17.168 | 69.256 | 1.00 | 39.49 |
| MOTA | 14041 | CG | TYR | 2112 | | -16.279 | 69.755 | | 41.55 |
| MOTA | 14042 | CD1 | TYR | 2112 | 27.152 | -16.250 | 69.101 | 1.00 | 42.17 |
| | | | | | | | | | |

| MOTA | 14043 | CE1 | TYR | 2112 | | 26,106 | -15.461 | 69.569 | 1.00 43.58 |
|------|-------|--------------|-----|------|---|--------|---------|------------------|------------|
| ATOM | 14044 | CD2 | TYR | 2112 | | | -15.488 | 70.897 | 1.00 42.83 |
| ATOM | 14045 | CE2 | TYR | 2112 | | | -14.695 | 71.374 | 1.00 43.95 |
| ATOM | 14046 | CZ | TYR | 2112 | | | -14.687 | 70.707 | 1.00 44.41 |
| | 14047 | OH | TYR | 2112 | | | -13.912 | 71.176 | 1.00 46.08 |
| ATOM | | | | 2112 | | | -18.190 | 69.761 | 1.00 37.30 |
| ATOM | 14048 | C | TYR | | | | | | |
| MOTA | 14049 | 0 | TYR | 2112 | | | -19.080 | 70.610 | 1.00 35.99 |
| ATOM | 14050 | N | LYS | 2113 | | 32.417 | -18.254 | 68.628 | 1.00 36.90 |
| MOTA | 14051 | CA | LYS | 2113 | | | -19.400 | 68.362 | 1.00 38.21 |
| MOTA | 14052 | CB | LYS | 2113 | | 33.784 | -19.378 | 66.914 | 1.00 36.95 |
| ATOM | 14053 | CG | LYS | 2113 | | 34.652 | -20.579 | 66.560 | 1.00 34.27 |
| ATOM | 14054 | CD | LYS | 2113 | | 34.828 | -20.750 | 65.061 | 1.00 32.97 |
| ATOM | 14055 | CE | LYS | 2113 | | 35.585 | -22.041 | 64.761 | 1.00 32.84 |
| ATOM | 14056 | NZ | LYS | 2113 | | 35.432 | -22.499 | 63.348 | 1.00 30.32 |
| ATOM | 14057 | С | LYS | 2113 | | | -19.411 | 69.328 | 1.00 38.99 |
| ATOM | 14058 | ō | LYS | 2113 | | | -20.471 | 69.782 | 1.00 38.16 |
| ATOM | 14059 | N | GLN | 2114 | | | -18.229 | 69.639 | 1.00 40.94 |
| ATOM | 14060 | CA | GLN | 2114 | | | -18.110 | 70.557 | 1.00 42.72 |
| | | | | 2114 | | | -16.653 | 70.652 | 1.00 44.16 |
| ATOM | 14061 | CB | GLN | | | | | 69.390 | 1.00 48.37 |
| ATOM | 14062 | CG | GLN | 2114 | | | -16.133 | | |
| MOTA | 14063 | CD | GLN | 2114 | | | -14.663 | 69.486 | 1.00 51.00 |
| MOTA | 14064 | OE1 | | 2114 | | | -14.254 | 70.386 | 1.00 53.01 |
| MOTA | 14065 | NE2 | GLN | 2114 | | | -13.861 | 68.551 | 1.00 51.71 |
| MOTA | 14066 | С | GLN | 2114 | | | -18.617 | 71.942 | 1.00 42.63 |
| ATOM | 14067 | 0 | GLN | 2114 | | 36.537 | -19.263 | 72.616 | 1.00 42.99 |
| ATOM | 14068 | N | GLU | 2115 | | 34.508 | -18.320 | 72.358 | 1.00 42.51 |
| ATOM | 14069 | CA | GLU | 2115 | | 34.016 | -18.745 | 73.664 | 1.00 42.44 |
| MOTA | 14070 | CB | GLU | 2115 | | 33.001 | -17.736 | 74.207 | 1.00 44.97 |
| ATOM | 14071 | CG | GLU | 2115 | | | -16.292 | 74.162 | 1.00 47.71 |
| ATOM | 14072 | CD | GLU | 2115 | | | -15.348 | 74.816 | 1.00 49.87 |
| MOTA | 14073 | OE1 | | 2115 | | | -15.405 | 74.472 | 1.00 50.50 |
| MOTA | 14074 | OE2 | | 2115 | | | -14.545 | 75.674 | 1.00 52.16 |
| | | C | | 2115 | | | -20.114 | 73.558 | 1.00 40.83 |
| MOTA | 14075 | | GLU | | | | | 74.532 | 1.00 40.05 |
| MOTA | 14076 | 0 | GLU | 2115 | | | -20.624 | | |
| MOTA | 14077 | N | LYS | 2116 | | | -20.701 | 72.368 | 1.00 39.34 |
| ATOM | 14078 | CA | LYS | 2116 | | | -22.010 | 72.130 | 1.00 38.09 |
| MOTA | 14079 | CB | LYS | 2116 | | | -23.079 | 72.923 | 1.00 40.37 |
| ATOM | 14080 | CG | LYS | 2116 | | | -23.210 | 72.540 | 1.00 42.96 |
| MOTA | 14081 | CD | LYS | 2116 | | 35.213 | -23.602 | 71.075 | 1.00 45.90 |
| ATOM | 14082 | CE | LYS | 2116 | | 36.679 | -23.631 | 70.646 | 1.00 47.03 |
| ATOM | 14083 | NZ | LYS | 2116 | | 37.471 | -24.671 | 71.351 | 1.00 46.52 |
| MOTA | 14084 | С | LYS | 2116 | | 31.332 | -22.042 | 72.493 | 1.00 36.61 |
| ATOM | 14085 | 0 | LYS | 2116 | | 30.836 | -23.016 | 73.062 | 1.00 35.86 |
| ATOM | 14086 | N | LYS | 2117 | | 30.620 | -20.972 | 72.159 | 1.00 35.40 |
| ATOM | 14087 | CA | LYS | 2117 | | | -20.908 | 72.444 | 1.00 33.94 |
| ATOM | 14088 | CB | LYS | 2117 | | | -19.570 | 73.100 | 1.00 34.82 |
| ATOM | 14089 | CG | LYS | 2117 | | | -19.354 | 73.271 | 1.00 36.44 |
| ATOM | 14090 | CD | LYS | 2117 | - | | -18.265 | 74.290 | 1.00 38.88 |
| | | | LYS | 2117 | | | -18.729 | 75.695 | 1.00 39.51 |
| ATOM | 14091 | CE | | | | | | - | 1.00 33.31 |
| MOTA | 14092 | NZ | LYS | 2117 | | | -17.658 | 76.714 71.166 | 1.00 41.13 |
| MOTA | 14093 | C | LYS | 2117 | | | -21.107 | | |
| MOTA | 14094 | 0 | LYS | 2117 | | | -20.232 | 70.300 | 1.00 31.72 |
| ATOM | 14095 | N | ARG | 2118 | | | -22.274 | 71.060 | 1.00 30.34 |
| MOTA | 14096 | CA | ARG | 2118 | | | -22.628 | 69.902 | 1.00 30.20 |
| MOTA | 14097 | CB | ARG | 2118 | | | -24.105 | 69.984 | 1.00 30.53 |
| MOTA | 14098 | CG | ARG | 2118 | | | -25.045 | 69.596 | 1.00 32.66 |
| MOTA | 14099 | CD | ARG | 2118 | | 27.360 | -26.506 | 69.872 | 1.00 33.98 |
| MOTA | 14100 | NE | ARG | 2118 | | 27.573 | -26.853 | 71.274 | 1.00 34.15 |
| ATOM | 14101 | cz | ARG | 2118 | | 27.601 | -28.097 | 71.741 | 1.00 33.23 |
| ATOM | 14102 | NH1 | ARG | 2118 | | 27.427 | -29.121 | 70.918 | 1.00 33.99 |
| ATOM | 14103 | NH2 | ARG | 2118 | | | -28.321 | 73.031 | 1.00 31.99 |
| MOTA | 14104 | С | ARG | 2118 | | | -21.734 | 69.800 | 1.00 28.50 |
| ATOM | 14105 | Ö | ARG | 2118 | | | -21.635 | 70.741 | 1.00 28.26 |
| ATOM | 14106 | N | PHE | 2119 | | | -21.089 | 68.647 | 1.00 27.02 |
| | | CA | PHE | 2119 | | | -20.171 | 68.403 | 1.00 27.02 |
| ATOM | 14107 | | | 2119 | | | -18.816 | 67.965 | 1.00 25.78 |
| MOTA | 14108 | CB | PHE | | | | | | |
| ATOM | 14109 | CG | PHE | 2119 | | | -18.883 | 66.710 | 1.00 28.65 |
| ATOM | 14110 | CD1 | PHE | 2119 | | | -18.742 | 65.457 | 1.00 27.88 |
| MOTA | 14111 | CD2 | PHE | 2119 | | | -19.110 | 66.779 | 1.00 27.56 |
| MOTA | 14112 | | PHE | 2119 | | | -18.821 | 64.294 | 1.00 29.01 |
| MOTA | 14113 | | PHE | 2119 | | 27.975 | -19.192 | 65.624 | 1.00 28.48 |
| MOTA | 14114 | CZ_{\perp} | PHE | 2119 | | 27.371 | -19.047 | 64.377 | 1.00 29.61 |
| MOTA | 14115 | С | PHE | 2119 | | | -20.693 | 67.351 | 1.00 24.24 |
| MOTA | 14116 | 0 | PHE | 2119 | | 23.861 | -21.375 | 66.404 | 1.00 20.96 |
| MOTA | 14117 | N | ALA | 2120 | | 22.186 | -20.365 | 67.515 | 1.00 23.46 |
| ATOM | 14118 | CA | ALA | 2120 | | 21.162 | -20.810 | 66.577 | 1.00 23.11 |
| ATOM | 14119 | СВ | ALA | 2120 | | | -21.175 | 67.343 | 1.00 25.46 |

| ATOM | 14120 | С | ALA | 2120 | 20.857 | -19.756 | 65.510 | 1.00 | 22.49 |
|--------------|----------------|------------|------------|--------------|----------------|--------------------|------------------|------|----------------|
| ATOM | 14121 | 0 | ALA | 2120 | 20.928 | -18.553 | 65.765 | 1.00 | 20.69 |
| ATOM | 14122 | N | THR | 2121 | | -20.225 | 64.309 | | 20.02 |
| ATOM | 14123 | CA | THR | 2121 | | -19.350 | 63.186 | | 21.26 |
| ATOM | 14124 | CB OG1 | THR THR | 2121 2121 | | -19.357 -18.930 | 62.125 62.734 | | 22.14 27.92 |
| ATOM ATOM | 14125 14126 | CG2 | THR | 2121 | | -18.424 | 60.985 | | 29.91 |
| ATOM | 14127 | C | THR | 2121 | | -19.922 | 62.577 | | 17.16 |
| ATOM | 14128 | Õ | THR | 2121 | | -21.104 | 62.731 | | 17.14 |
| ATOM | 14129 | N | ILE | 2122 | | -19.102 | 61.885 | 1.00 | 18.16 |
| ATOM | 14130 | CA | ILE | 2122 | | -19.608 | 61.308 | | 16.98 |
| ATOM | 14131 | CB | ILE | 2122 | | -19.454 | 62.321 | | 19.66 |
| MOTA | 14132 | CG2 | ILE | 2122 | | -17.977 | 62.470 | | 18.99 20.97 |
| MOTA MOTA | 14133 14134 | CG1 CD1 | ILE ILE | 2122 2122 | | -20.260 -20.310 | 61.856 62.873 | | 23.87 |
| ATOM | 14135 | C | ILE | 2122 | | -18.882 | 60.020 | | 16.60 |
| ATOM | 14136 | ō | ILE | 2122 | | -17.772 | 59.792 | | 17.43 |
| MOTA | 14137 | N | THR | 2123 | 15.743 | -19.513 | 59.166 | 1.00 | 18.07 |
| MOTA | 14138 | CA | THR | 2123 | | -18.866 | 57.923 | | 17.40 |
| MOTA | 14139 | CB | THR | 2123 | | -19.892 | 56.836 | | 19.53 |
| MOTA | 14140 | OG1 | THR | 2123 | | -20.612 | 57.278 | | 20.71 |
| MOTA | 14141 | CG2 | THR THR | 2123 | | -20.876 -17.973 | 56.547 58.229 | | 19.80 16.12 |
| MOTA MOTA | 14142 14143 | C 0 | THR | 2123 2123 | | -18.244 | 59.152 | | 17.78 |
| ATOM | 14144 | N | ALA | 2124 | | -16.903 | 57.459 | | 16.44 |
| ATOM | 14145 | CA | ALA | 2124 | | -15.976 | 57.646 | | 15.59 |
| ATOM | 14146 | CB | ALA | 2124 | | -14.918 | 58.685 | | 17.03 |
| ATOM | 14147 | С | ALA. | 2124 | 12.600 | -15.330 | 56.291 | 1.00 | 14.67 |
| MOTA | 14148 | 0 | ALA | 2124 | | -15.046 | 55.556 | | 13.64 |
| ATOM | 14149 | N | TYR | 2125 | | -15.107 | 55.956 | | 13.33 |
| ATOM | 14150 | CA | TYR | 2125 | | -14.521 | 54.659 | | 12.55 |
| MOTA | 14151 | CB | TYR | 2125 2125 | | -15.599 -16.926 | 53.712 53.797 | | 14.08 13.16 |
| ATOM ATOM | 14152 14153 | CG . | TYR | 2125 | | -18.007 | 54.464 | | 15.20 |
| ATOM | 14154 | CE1 | TYR | 2125 | | -19.220 | 54.578 | | 19.44 |
| ATOM | 14155 | CD2 | TYR | 2125 | | -17.090 | 53.240 | | 15.12 |
| MOTA | 14156 | CE2 | TYR | 2125 | 13.122 | -18.308 | 53.351 | 1.00 | 16.49 |
| MOTA | 14157 | CZ | TYR | 2125 | | -19.362 | 54.023 | | 17.45 |
| ATOM | 14158 | OH | TYR | 2125 | | -20.559 | 54.160 | | 18.95 |
| ATOM | 14159 | C | TYR | 2125 | | -13.401 | 54.752 | | 14.84 |
| ATOM | 14160 | O | TYR ASP | 2125 2126 | | -12.876 -13.030 | 53.726 55.967 | | 13.18 15.18 |
| ATOM ATOM | 14161 14162 | N CA | ASP | 2126 | | -11.969 | 56.114 | | 15.35 |
| MOTA | 14163 | CB | ASP | 2126 | | -12.552 | 55.980 | | 16.11 |
| MOTA | 14164 | CG | ASP | 2126 | | -13.517 | 57.105 | | 17.38 |
| MOTA | 14165 | OD1 | ASP | 2126 | 6.660 | -13.064 | 58.256 | | 17.19 |
| MOTA | 14166 | OD2 | ASP | 2126 | | -14.729 | 56.837 | | 17.99 |
| MOTA | 14167 | C | ASP | 2126 | | -11.166 | 57.410 | | 16.68 |
| ATOM | 14168 | 0 | ASP | 2126 | | -11.549 | 58.325 | | 15.28 15.28 |
| ATOM ATOM | 14169 14170 | N CA | TYR TYR | 2127 2127 | 8.120 | -10.038 -9.164 | 57.475 58.641 | | 17.17 |
| ATOM | 14171 | CB | TYR | 2127 | 7.276 | | 58.397 | | 17.79 |
| ATOM | 14172 | CG | TYR | 2127 | 6.992 | -7.109 | 59.641 | | 17.73 |
| MOTA | 14173 | | TYR | 2127 | 7.875 | -6.122 | 60.075 | 1.00 | 20.38 |
| ATOM | 14174 | CE1 | TYR | 2127 | 7.605 | -5.367 | 61.218 | | 20.48 |
| MOTA | 14175 | CD2 | TYR | 2127 | 5.832 | -7.331 | 60.379 | | 20.09 |
| MOTA | 14176 | CE2 | TYR | 2127 | 5.551 | -6.590 | 61.519 | | 22.06 23.04 |
| ATOM | 14177 | CZ | TYR | 2127 | 6.439 6.152 | -5.610 -4.857 | 61.930 63.050 | | 24.49 |
| ATOM ATOM | 14178 14179 | OH C | TYR TYR | 2127 2127 | 7.671 | -4.837 -9.827 | 59.937 | | 18.30 |
| ATOM | 14180 | ō | TYR | 2127 | 8.354 | -9.732 | 60.961 | | 17.92 |
| ATOM | 14181 | N | SER | 2128 | | -10.487 | 59.886 | | 19.07 |
| ATOM | 14182 | CA | SER | 2128 | 5.943 | -11.136 | 61.055 | | 21.09 |
| MOTA | 14183 | CB | SER | 2128 | | -11.836 | 60.682 | | 22.18 |
| MOTA | 14184 | OG | SER | 2128 | | -10.872 | 60.424 | | 21.45 |
| ATOM | 14185 | C | SER | 2128 | | -12.120 | 61.754 | | 21.26 20.52 |
| ATOM | 14186 | O | SER | 2128 2129 | | -11.960 -13.143 | 62.943 61.036 | | 18.91 |
| MOTA MOTA | 14187 14188 | N CA | PHE PHE | , | | -13.143 | 61.661 | | 18.72 |
| MOTA | 14189 | CB | PHE | 2129 | | -15.338 | 60.770 | | 19.49 |
| ATOM | 14190 | CG | PHE | 2129 | | -16.303 | 60.797 | | 20.01 |
| ATOM | 14191 | CD1 | PHE | 2129 | | -16.317 | 59.772 | 1.00 | 18.47 |
| MOTA | 14192 | CD2 | PHE | 2129 | | -17.186 | 61.862 | | 19.74 |
| MOTA | 14193 | | PHE | 2129 | | -17.198 | 59.811 | | 19.85 |
| MOTA | 14194 | CE2 | PHE | 2129 | | -18.067 | 61.907 | | 20.86 |
| ATOM. | 14195 | cz | PHE | | | -18.076 -13.489 | 60.879 62.039 | | 20.11 17.47 |
| ATOM | 14196 | С | PHE | 2129 | 9.341 | - TJ . #07 | 02.033 | 2.00 | 1,.3/ |
| | | | | | | | | | |

| ATOM | 14197 | 0 | PHE | 2129 | 10.064 -13.79 | 63.097 | 1.00 19.2 | 6 |
|--------|----------------|-----|-----|------|----------------|--------------|-----------|---|
| ATOM | 14198 | N | ALA | 2130 | 10.055 -12.59 | | 1.00 18.9 | |
| ATOM | 14199 | CA | ALA | 2130 | 11.333 -11.95 | | 1.00 17.7 | |
| ATOM | 14200 | CB | ALA | 2130 | 11.724 -11.00 | | 1.00 17.9 | |
| ATOM | 14201 | C | ALA | 2130 | 11.247 -11.20 | | 1.00 20.3 | |
| АТОМ | 14202 | 0 | ALA | 2130 | 12.143 -11.28 | | 1.00 17.9 | |
| ATOM | 14203 | N | LYS | 2131 | 10.156 -10.46 | | 1.00 19.4 | |
| ATOM | 14204 | CA | LYS | 2131 | 9.932 -9.69 | | 1.00 22.3 | |
| ATOM | 14205 | CB | LYS | 2131 | 8.625 -8.90 | | 1.00 23.8 | |
| ATOM | 14206 | CG | LYS | 2131 | 8.301 -7.97 | | 1.00 26.4 | |
| ATOM | 14207 | CD | LYS | 2131 | 9.254 -6.79 | | 1.00 29.9 | |
| ATOM | 14208 | CE | LYS | 2131 | 8.767 -5.71 | | 1.00 30.6 | |
| ATOM | 14209 | NZ | LYS | 2131 | 8.650 -6.21 | | 1.00 32.0 | |
| ATOM | 14210 | C | LYS | 2131 | 9.861 -10.62 | | 1.00 21.6 | |
| ATOM | 14211 | ō | LYS | 2131 | 10.447 -10.35 | | 1.00 24.2 | |
| ATOM | 14212 | N | LEU | 2132 | 9.149 -11.73 | | 1.00 20.4 | |
| ATOM | 14213 | CA | LEU | 2132 | 8.981 -12.71 | | 1.00 21.7 | |
| ATOM | 14214 | CB | LEU | 2132 | 8.000 -13.80 | | 1.00 20.3 | |
| MOTA | 14215 | CG | LEU | 2132 | 7.523 -14.83 | | 1.00 21.9 | |
| ATOM | 14216 | CD1 | | 2132 | 6.279 -15.52 | | 1.00 21.2 | |
| ATOM | 14217 | | LEU | 2132 | 8.608 -15.86 | | 1.00 19.4 | |
| ATOM | 14218 | C | LEU | 2132 | 10.303 -13.33 | | 1.00 21.6 | |
| ATOM | 14219 | ō | LEU | 2132 | 10.524 -13.57 | | 1.00 20.1 | |
| ATOM | 14220 | N | PHE | 2133 | 11.177 -13.61 | | 1.00 20.3 | |
| ATOM | 14221 | CA | PHE | 2133 | 12.474 -14.20 | | 1.00 20.0 | |
| ATOM | 14222 | CB | PHE | 2133 | 13.196 -14.65 | | 1.00 18.1 | |
| ATOM · | 14223 | CG | PHE | 2133 | 12.452 -15.69 | | 1.00 15.7 | |
| ATOM | 14224 | CD1 | | 2133 | 11.618 -16.61 | | 1.00 15.9 | |
| ATOM | 14225 | CD2 | PHE | 2133 | 12.598 -15.77 | | 1.00 16.4 | |
| ATOM | 14226 | CE1 | PHE | 2133 | 10.934 -17.58 | | 1.00 17.0 | |
| ATOM | 14227 | CE2 | PHE | 2133 | 11.922 -16.74 | | 1.00 13.6 | |
| ATOM | 14228 | CZ | PHE | 2133 | 11.087 -17.65 | | 1.00 15.9 | |
| ATOM | 14229 | C | PHE | 2133 | 13.344 -13.21 | | 1.00 20.4 | |
| ATOM | 14230 | 0 | PHE | 2133 | 13.940 -13.54 | | 1.00 22.6 | |
| ATOM | 14231 | N | ALA | 2134 | 13.420 -11.99 | | 1.00 20.9 | |
| ATOM | 14232 | CA | ALA | 2134 | 14.230 -10.95 | | 1.00 22.5 | |
| ATOM | 14233 | CB | ALA | 2134 | 14.139 -9.67 | | 1.00 22.9 | |
| ATOM | 14234 | C | ALA | 2134 | 13.799 -10.69 | | 1.00 25.2 | |
| ATOM | 14235 | ō | ALA | 2134 | 14.636 -10.47 | | 1.00 25.7 | |
| ATOM | 14236 | N | ASP | 2135 | 12.494 -10.71 | | 1.00 24.8 | |
| ATOM | 14237 | CA | ASP | 2135 | 12.001 -10.47 | | 1.00 27.3 | |
| ATOM | 14238 | СВ | ASP | 2135 | 10.489 -10.24 | | 1.00 28.3 | |
| ATOM | 14239 | CG | ASP | 2135 | 10.086 -8.97 | | 1.00 28.7 | |
| ATOM | 14240 | | ASP | 2135 | 10.963 -8.13 | | 1.00 29.2 | |
| ATOM | 14241 | OD2 | ASP | 2135 | 8.876 -8.80 | | 1.00 28.6 | |
| ATOM | 14242 | C | ASP | 2135 | 12.334 -11.59 | | 1.00 27.1 | |
| ATOM | 14243 | 0 | ASP | 2135 | 12.518 -11.34 | | 1.00 26.0 | |
| ATOM | 14244 | N | GLU | 2136 | 12.406 -12.82 | | 1.00 27.9 | |
| MOTA | 14245 | CA | GLU | 2136 | 12.708 -13.96 | | 1.00 28.8 | |
| ATOM | 14246 | CB | GLU | 2136 | 12.111 -15.24 | | 1.00 27.5 | |
| ATOM | 14247 | CG | GLU | 2136 | 10.611 -15.24 | | 1.00 30.4 | |
| ATOM | 14248 | CD | GLU | 2136 | 10.063 -14.819 | | 1.00 31.3 | |
| ATOM | 14249 | | GLU | 2136 | 10.393 -15.49 | | 1.00 32.3 | |
| ATOM | 14250 | | GLU | 2136 | 9.319 -13.810 | | 1.00 28.1 | |
| ATOM | 14251 | C | GLU | 2136 | 14.187 -14.17 | | 1.00 29.3 | |
| ATOM | 14252 | o | GLU | 2136 | 14.567 -14.89 | | 1.00 30.7 | |
| ATOM | 14253 | N | GLY | 2137 | 15.029 -13.58 | | 1.00 30.4 | |
| ATOM | 14254 | CA | GLY | 2137 | 16.461 -13.73 | | 1.00 30.6 | |
| ATOM | 14255 | C | GLY | 2137 | 17.255 -14.11 | | 1.00 29.3 | |
| ATOM | 14256 | ō | GLY | 2137 | 18.475 -13.97 | | 1.00 28.3 | |
| ATOM | 14257 | N | LEU | 2138 | 16.572 -14.60 | | 1.00 28.3 | |
| ATOM | 14258 | CA | LEU | 2138 | 17.229 -15.00 | | 1.00 26.9 | |
| ATOM | 14259 | СВ | LEU | 2138 | 16.304 -15.88 | | 1.00 28.3 | |
| ATOM | 14260 | CG | LEU | 2138 | 16.435 -17.38 | | 1.00 27.7 | |
| ATOM | 14261 | | LEU | 2138 | 15.372 -18.12 | | 1.00 24.2 | |
| ATOM | 14262 | | LEU | 2138 | 17.826 -17.82 | | 1.00 29.1 | |
| ATOM | 14263 | C | LEU | 2138 | 17.590 -13.76 | | 1.00 27.2 | |
| ATOM | 14264 | o | LEU | 2138 | 16.708 -13.06 | | 1.00 27.9 | |
| ATOM | 14265 | N | ASN | 2139 | 18.886 -13.50 | | 1.00 24.3 | |
| ATOM | 14266 | CA | ASN | 2139 | 19.344 -12.33 | | 1.00 23.7 | |
| ATOM | 14267 | CB | ASN | 2139 | 20.224 -11.46 | | 1.00 27.7 | |
| ATOM | 14268 | CG | ASN | 2139 | 19.509 -11.020 | | 1.00 31.1 | |
| ATOM | 14269 | | ASN | 2139 | 18.415 -10.458 | | 1.00 34.0 | |
| ATOM | 14270 | | ASN | 2139 | 20.125 -11.279 | | 1.00 33.2 | |
| ATOM | 14271 | C | ASN | 2139 | 20.112 -12.66 | | 1.00 20.1 | |
| MOTA | 14272 | o | ASN | 2139 | 20.800 -11.804 | | 1.00 21.0 | |
| ATOM | 14273 | N | VAL | 2140 | 20.020 -13.90 | | 1.00 17.9 | |
| | · - | | | | | - | | |

| MOTA | 14274 | CA | VAL | 2140 | 20.703 | -14.304 | 62.860 | 1.00 17.14 |
|------|-------|-----|-----|--------|--------|---------|--------|------------|
| ATOM | 14275 | CB | VAL | 2140 | 21.860 | -15.287 | 63.124 | 1.00 19.66 |
| ATOM | 14276 | CG1 | | 2140 | | -15.512 | 61.834 | 1.00 17.34 |
| | | | | | | | | 1.00 21.32 |
| MOTA | 14277 | | VAL | 2140 | | -14.735 | 64.215 | |
| MOTA | 14278 | С | VAL | 2140 | | -14.991 | 61.969 | 1.00 14.62 |
| ATOM | 14279 | 0 | VAL | 2140 | 19.224 | -16.085 | 62.273 | 1.00 14.94 |
| ATOM | 14280 | N | MET | 2141 | 19.324 | -14.338 | 60.872 | 1.00 15.56 |
| ATOM | 14281 | CA | MET | 2141 | 18.332 | -14.888 | 59.971 | 1.00 15.34 |
| ATOM | 14282 | СВ | MET | 2141 | | -14.034 | 60.024 | 1.00 17.74 |
| | | | | | | | | 1.00 20.01 |
| MOTA | 14283 | CG | MET | 2141 | | -14.068 | 61.383 | |
| MOTA | 14284 | SD | MET | 2141 | | -12.883 | 61.483 | 1.00 22.65 |
| ATOM | 14285 | CE | MET | 2141 | 15.531 | -11.942 | 62.941 | 1.00 20.39 |
| ATOM | 14286 | С | MET | 2141 | 18.827 | -14.989 | 58.548 | 1.00 14.81 |
| ATOM | 14287 | 0 | MET | 2141 | 19.577 | -14.136 | 58.069 | 1.00 14.45 |
| ATOM | 14288 | N | LEU | 2142 | 18.393 | -16.040 | 57.869 | 1.00 15.04 |
| ATOM | 14289 | CA | LEU | 2142 | | -16.250 | 56.483 | 1.00 15.97 |
| | | | | | | -17.609 | 56.352 | 1.00 17.78 |
| MOTA | 14290 | CB | LEU | 2142 | | | | |
| MOTA | 14291 | CG | LEU | 2142 | | -18.146 | 54.997 | 1.00 23.22 |
| MOTA | 14292 | CD1 | LEU | 2142 | | -18.861 | 54.306 | 1.00 25.80 |
| MOTA | 14293 | CD2 | LEU | 2142 | 20.536 | -17.032 | 54.136 | 1.00 22.00 |
| MOTA | 14294 | C | LEU | 2142 | 17.555 | -16.182 | 55.572 | 1.00 14.69 |
| ATOM | 14295 | 0 | LEU | 2142 | 16,570 | -16.886 | 55.781 | 1.00 14.54 |
| ATOM | 14296 | N | VAL | 2143 | | -15.299 | 54.582 | 1.00 13.79 |
| | | | | 2143 | | -15.156 | 53.596 | 1.00 14.55 |
| MOTA | 14297 | CA | VAL | | | -13.136 | 53.162 | 1.00 14.33 |
| ATOM | 14298 | CB | VAL | 2143 | | | | |
| ATOM | 14299 | CG1 | | 2143 | | -13.584 | 52.093 | 1.00 17.16 |
| MOTA | 14300 | CG2 | VAL | 2143 | 16.006 | -12.837 | 54.379 | 1.00 16.68 |
| ATOM | 14301 | С | VAL | 2143 | 17.126 | -15.985 | 52.450 | 1.00 14.62 |
| ATOM | 14302 | 0 | VAL | 2143 | 17.824 | -15.466 | 51.583 | 1.00 15.21 |
| ATOM | 14303 | N | GLY | 2144 | | -17.283 | 52.474 | 1.00 16.51 |
| ATOM | 14304 | CA | | 2144 | | -18.166 | 51.454 | 1.00 16.80 |
| | | | GLY | | | | | 1.00 16.58 |
| ATOM | 14305 | С | GLY | 2144 | | -18.554 | 50.339 | |
| MOTA | 14306 | 0 | GLY | 2144 | | -18.396 | 50.455 | 1.00 15.97 |
| MOTA | 14307 | N | ASP | 2145 | 17.009 | -19.077 | 49.254 | 1.00 15.26 |
| MOTA | 14308 | CA | ASP | 2145 | 16.193 | -19.474 | 48.107 | 1.00 16.47 |
| MOTA | 14309 | CB | ASP | 2145 | 17.066 | -19.746 | 46.875 | 1.00 16.11 |
| ATOM | 14310 | CG | ASP | 2145 | | -20.849 | 47.095 | 1.00 17.05 |
| ATOM | 14311 | | ASP | 2145 | | -21.434 | 48.182 | 1.00 15.53 |
| | | | | | | | | |
| ATOM | 14312 | OD2 | ASP | 2145 | | -21.122 | 46.159 | 1.00 20.23 |
| MOTA | 14313 | C | ASP | 2145 | | -20.667 | 48.406 | 1.00 14.31 |
| MOTA | 14314 | Ο. | ASP | 2145 | 14.536 | -21.124 | 47.542 | 1.00 13.80 |
| ATOM | 14315 | N | SER | 2146 | 15.350 | -21.158 | 49.642 | 1.00 15.43 |
| MOTA | 14316 | CA | SER | 2146 | 14.475 | -22.251 | 50.051 | 1.00 13.71 |
| ATOM | 14317 | CB | SER | 2146 | 14.764 | -22.668 | 51.498 | 1.00 14.86 |
| ATOM | 14318 | OG | SER | 2146 | | -21.562 | 52.384 | 1.00 15.94 |
| | | | | | | -21.724 | 49.938 | 1.00 13.48 |
| MOTA | 14319 | C | SER | | | | | |
| ATOM | 14320 | 0 | SER | 2146 | | -22.493 | 49.838 | 1.00 13.05 |
| MOTA | 14321 | N | LEU | 2147 | | -20.403 | 49.960 | 1.00 13.53 |
| MOTA | 14322 | CA | LEU | 2147 | 11.580 | -19.798 | 49.848 | 1.00 15.06 |
| ATOM | 14323 | CB | LEU | 2147 | 11.676 | -18.270 | 49.964 | 1.00 14.88 |
| ATOM | 14324 | CG | LEU | 2147 | 12.398 | -17.474 | 48.868 | 1.00 15.50 |
| ATOM | 14325 | CD1 | LEU | 2147 | 11.425 | -17.211 | 47.718 | 1.00 12.97 |
| ATOM | 14326 | | LEU | 2147 | | -16.144 | 49.442 | 1.00 14.61 |
| ATOM | 14327 | CDZ | LEU | 2147 | | -20.193 | 48.532 | 1.00 15.02 |
| | | | | | | | | |
| ATOM | 14328 | 0 | LEU | 2147 | | -20.120 | 48.406 | 1.00 13.70 |
| ATOM | 14329 | N | GLY | 2148 | | -20.618 | 47.556 | 1.00 13.80 |
| ATOM | 14330 | CA | GLY | 2148 | | -21.027 | 46.282 | 1.00 14.73 |
| MOTA | 14331 | С | GLY | 2148 | 10.168 | -22.193 | 46.449 | 1.00 15.52 |
| MOTA | 14332 | 0 | GLY | 2148 | 9.240 | -22.374 | 45.664 | 1.00 15.06 |
| ATOM | 14333 | N | MET | 2149 | | -22.984 | 47.490 | 1.00 16.51 |
| ATOM | 14334 | CA | MET | 2149 | 9.543 | -24.142 | 47.739 | 1.00 18.26 |
| | | CB | MET | 2149 | | -25.344 | 48.105 | 1.00 19.59 |
| MOTA | 14335 | | | | | | | |
| MOTA | 14336 | CG | MET | 2149 | 11.372 | -25.737 | 46.979 | 1.00 23.21 |
| MOTA | 14337 | SD | MET | 2149 | | -27.009 | 47.403 | 1.00 26.89 |
| MOTA | 14338 | CE | MET | 2149 · | | -28.406 | 47.735 | 1.00 27.42 |
| ATOM | 14339 | С | MET | 2149 | 8.525 | -23.867 | 48.836 | 1.00 17.57 |
| MOTA | 14340 | 0 | MET | 2149 | | -24.072 | 48.643 | 1.00 18.80 |
| ATOM | 14341 | N | THR | 2150 | | -23.374 | 49.974 | 1.00 17.41 |
| ATOM | 14342 | CA | THR | 2150 | | -23.094 | 51.106 | 1.00 19.06 |
| | | | | | | -22.896 | 52.395 | 1.00 10.00 |
| MOTA | 14343 | CB | THR | 2150 | | | | |
| ATOM | 14344 | OG1 | THR | 2150 | | -22.760 | 53.500 | 1.00 28.01 |
| MOTA | 14345 | CG2 | THR | 2150 | | -21.652 | 52.296 | 1.00 16.62 |
| MOTA | 14346 | С | THR | 2150 | | -21.893 | 50.948 | 1.00 19.09 |
| ATOM | 14347 | 0 | THR | 2150 | 6.085 | -21.890 | 51.495 | 1.00 19.04 |
| ATOM | 14348 | N | VAL | 2151 | | -20.878 | 50.212 | 1.00 15.32 |
| ATOM | 14349 | CA | VAL | 2151 | | -19.688 | 50.000 | 1.00 15.78 |
| ATOM | | | | | | -18.400 | 50.167 | 1.00 13.78 |
| ATOM | 14350 | СВ | VAL | 2151 | 7.000 | -10.400 | 30.107 | 1.00 14.07 |
| | | | | | | | | |

| ATOM | 14351 | CG1 | VAL | 2151 | 6.850 | -17.167 | 49.740 | 1.00 14.82 |
|--------|-------|-----|-------|------|--------|---------|--------|------------|
| ATOM | 14352 | CG2 | VAL | 2151 | 8 092 | -18.258 | 51.629 | 1.00 16.78 |
| | 14353 | C | VAL | 2151 | | -19.683 | 48.634 | 1.00 15.00 |
| ATOM | | | | | | | | |
| MOTA | 14354 | 0 | VAL | 2151 | | -19.573 | 48.554 | 1.00 12.68 |
| ATOM | 14355 | N | GLN | 2152 | 6.898 | -19.827 | 47.562 | 1.00 12.81 |
| ATOM | 14356 | CA | GLN | 2152 | 6.332 | -19.819 | 46.205 | 1.00 12.29 |
| ATOM | 14357 | СВ | GLN | 2152 | | -19.435 | 45.195 | 1.00 9.78 |
| | | | | | | | | |
| MOTA | 14358 | CG | GLN | 2152 | | -18.150 | 45.545 | 1.00 11.69 |
| MOTA | 14359 | CD | GLN | 2152 | | -17.866 | 44.616 | 1.00 12.80 |
| MOTA | 14360 | OE1 | GLN | 2152 | 9.733 | -18.750 | 43.901 | 1.00 13.02 |
| MOTA | 14361 | NE2 | GLN | 2152 | 9.765 | -16.630 | 44.639 | 1.00 10.46 |
| ATOM | 14362 | C | GLN | 2152 | | -21.127 | 45.773 | 1.00 13.36 |
| | | | | | | | | |
| MOTA | 14363 | 0 | GLN | 2152 | | -21.127 | 44.897 | 1.00 13.82 |
| MOTA | 14364 | N | GLY | 2153 | | -22.244 | 46.368 | 1.00 14.36 |
| ATOM | 14365 | CA | GLY | 2153 | 5.485 | -23.517 | 46.020 | 1.00 13.48 |
| ATOM | 14366 | С | GLY | 2153 | 6.071 | -24.295 | 44.852 | 1.00 14.85 |
| ATOM | 14367 | 0 | GLY | 2153 | 5 409 | -25.187 | 44.308 | 1.00 13.64 |
| | | | | | | -23.974 | 44.464 | 1.00 14.25 |
| MOTA | 14368 | N | HIS | 2154 | | | | |
| MOTA | 14369 | CA | HIS | 2154 | | -24.675 | 43.362 | 1.00 16.22 |
| MOTA | 14370 | CB | HIS | 2154 | 9.061 | -23.799 | 42.755 | 1.00 14.89 |
| ATOM | 14371 | CG | HIS | 2154 | 8.556 | -22.555 | 42.100 | 1.00 16.52 |
| MOTA | 14372 | CD2 | HIS | 2154 | 8.719 | -21.251 | 42.426 | 1.00 15.21 |
| ATOM | 14373 | | HIS | 2154 | | -22.572 | 40.949 | 1.00 16.03 |
| | | | | | | | | |
| MOTA | 14374 | | HIS | 2154 | | -21.332 | 40.595 | 1.00 18.56 |
| MOTA | 14375 | | HIS | 2154 | | -20.512 | 41.474 | 1.00 18.50 |
| MOTA | 14376 | С | HIS | 2154 | 8.586 | -25.991 | 43.836 | 1.00 17.17 |
| ATOM | 14377 | 0 | HIS | 2154 | 8.770 | -26.202 | 45.032 | 1.00 17.56 |
| ATOM | 14378 | N | ASP | 2155 | | -26.868 | 42.889 | 1.00 18.27 |
| | | | | | | | 43.211 | |
| ATOM | 14379 | CA | ASP | 2155 | | -28.163 | | |
| MOTA | 14380 | CB | ASP | 2155 | | -29.141 | 42.041 | 1.00 26.36 |
| ATOM | 14381 | CG | ASP | 2155 | 10.020 | -28.659 | 40.771 | 1.00 30.40 |
| ATOM | 14382 | OD1 | ASP | 2155 | 11.238 | -28.378 | 40.795 | 1.00 35.46 |
| MOTA | 14383 | OD2 | ASP | 2155 | 9.331 | -28.562 | 39.727 | 1.00 38.63 |
| ATOM | 14384 | C | ASP | 2155 | | -28.060 | 43.568 | 1.00 18.34 |
| | 14385 | ō | ASP | 2155 | | -29.037 | 43.990 | 1.00 19.68 |
| ATOM | | | | | | | | |
| MOTA | 14386 | N | SER | 2156 | | -26.878 | 43.387 | |
| MOTA | 14387 | CA | SER | 2156 | | -26.667 | 43.692 | 1.00 14.88 |
| MOTA | 14388 | CB | SER | 2156 | | -27.160 | 42.535 | 1.00 15.97 |
| ATOM | 14389 | OG | SER | 2156 | 13.813 | -26.262 | 41.438 | 1.00 12.59 |
| MOTA | 14390 | С | SER | 2156 | 13.215 | -25.187 | 43.923 | 1.00 15.41 |
| MOTA | 14391 | 0 | SER | 2156 | 12,300 | -24.372 | 43.791 | 1.00 14.28 |
| ATOM | 14392 | N | THR | 2157 | | -24.833 | 44.263 | 1.00 13.49 |
| | 14393 | CA | THR | 2157 | | -23.433 | 44.514 | 1.00 14.04 |
| ATOM | | | | | | | | |
| MOTA | 14394 | СВ | THR | 2157 | | -23.292 | 45.558 | 1.00 14.05 |
| ATOM | 14395 | OG1 | | 2157 | | -23.825 | 45.018 | 1.00 16.03 |
| ATOM | 14396 | CG2 | THR | 2157 | 15.550 | -24.034 | 46.839 | 1.00 16.22 |
| ATOM | 14397 | C | THR | 2157 | 15.219 | -22.668 | 43.270 | 1.00 13.58 |
| ATOM | 14398 | 0 | THR | 2157 | 15.329 | -21.440 | 43.313 | 1.00 12.41 |
| ATOM | 14399 | N | LEU | 2158 | 15:450 | -23.374 | 42.162 | 1.00 13.34 |
| ATOM | 14400 | CA | LEU | 2158 | | -22.722 | 40.937 | 1.00 12.31 |
| | | | | | | | | |
| MOTA | 14401 | CB | LEU | 2158 | | -23.761 | 39.808 | 1.00 14.42 |
| MOTA | 14402 | CG | LEU | 2158 | 17.337 | -24.646 | 39.959 | 1.00 16.63 |
| ATOM | 14403 | CD1 | LEU | 2158 | 17.106 | -25.616 | 41.104 | 1.00 17.91 |
| ATOM | 14404 | CD2 | LEU | 2158 | 17.631 | -25.409 | 38.669 | 1.00 18.40 |
| ATOM | 14405 | С | LEU | 2158 | | -21.500 | 40.413 | 1.00 12.03 |
| | | | | | | -20.523 | 40.004 | 1.00 11.95 |
| MOTA | 14406 | 0 | LEU | 2158 | | | | |
| MOTA | 14407 | N | PRO | 2159 | | -21.526 | 40.437 | 1.00 11.73 |
| MOTA | 14408 | CD | PRO | 2159 | | -22.627 | 40.802 | 1.00 13.77 |
| MOTA | 14409 | CA | PRO | 2159 | 13.060 | -20.378 | 39.941 | 1.00 11.00 |
| ATOM | 14410 | CB | PRO | 2159 | 11.629 | -20.913 | 39.914 | 1.00 13.29 |
| MOTA | 14411 | CG | PRO | 2159 | 11.619 | -21.891 | 41.005 | 1.00 17.80 |
| MOTA | 14412 | C | PRO | 2159 | | -19.078 | 40.737 | 1.00 8.57 |
| | 14413 | | | 2159 | | -18.016 | 40.253 | 1.00 10.80 |
| ATOM | | 0 | PRO | | | | | |
| ATOM | 14414 | N | VAL | 2160 | | -19.147 | 41.949 | 1.00 9.75 |
| ATOM | 14415 | CA | VAL | 2160 | | -17.939 | 42.764 | 1.00 10.64 |
| MOTA | 14416 | CB | VAL | 2160 | | -18.295 | 44.191 | 1.00 7.98 |
| MOTA | 14417 | CG1 | VAL | 2160 | 14.487 | -17.023 | 45.046 | 1.00 8.99 |
| ATOM | 14418 | CG2 | VAL | 2160 | 13.339 | -19.249 | 44.833 | 1.00 9.25 |
| ATOM | 14419 | С | VAL | 2160 | | -16.956 | 42.120 | 1.00 10.30 |
| ATOM | 14420 | Ö | VAL | 2160 | | -17.302 | 41.812 | 1.00 12.24 |
| | | | | | | -15.718 | 41.940 | 1.00 12.24 |
| MOTA | 14421 | N | THR | 2161 | | | | |
| MOTA | 14422 | CA | THR | 2161 | | -14.686 | 41.310 | 1.00 13.51 |
| MOTA | 14423 | CB | THR | 2161 | | -13.853 | 40.324 | 1.00 17.26 |
| MOTA | 14424 | OG1 | THR | 2161 | 13.616 | -14.733 | 39.449 | 1.00 18.29 |
| ATOM | 14425 | CG2 | THR | 2161 | 15.234 | -12.954 | 39.478 | 1.00 19.77 |
| ATOM | 14426 | C | THR | 2161 | | -13.747 | 42.335 | 1.00 10.55 |
| ATOM | 14427 | ō | THR | 2161 | | -13.755 | 43.496 | 1.00 11.77 |
| 111011 | 12361 | J | ***** | 2101 | 10.41 | 13.733 | 15.470 | |
| | | | | | | | | |

| ATOM | 14428 | N | VAL | 2162 | 16.777 | -12.940 | 41.897 | 1.00 12.13 |
|--------------|-------|-----|-----|------|--------|---------|--------|------------|
| ATOM | 14429 | CA | VAL | 2162 | | -11.979 | 42.778 | 1.00 13.71 |
| ATOM | 14430 | СВ | VAL | 2162 | | -11.216 | 42.019 | 1.00 15.08 |
| ATOM | 14431 | | VAL | 2162 | | -10.057 | 42.858 | 1.00 16.93 |
| MOTA | 14432 | CG2 | | 2162 | | -12.172 | 41.676 | 1.00 15.68 |
| ATOM | 14433 | C | VAL | 2162 | | -11.000 | 43.310 | 1.00 13.50 |
| MOTA | 14434 | Ō | VAL | 2162 | | -10.571 | 44.469 | 1.00 14.68 |
| ATOM | 14435 | N | ALA | 2163 | | -10.662 | 42.455 | 1.00 13.50 |
| ATOM | 14436 | CA | ALA | 2163 | 14.352 | -9.751 | 42.827 | 1.00 12.58 |
| ATOM | 14437 | CB | ALA | 2163 | 13.454 | -9.473 | 41.606 | 1.00 13.55 |
| ATOM | 14438 | C | ALA | 2163 | | -10.352 | 43.956 | 1.00 12.11 |
| | 14439 | o | ALA | 2163 | 13.094 | -9.637 | 44.872 | 1.00 10.50 |
| ATOM ATOM | 14440 | N | ASP | 2164 | | -11.664 | 43.886 | 1.00 10.69 |
| ATOM | 14441 | CA | ASP | 2164 | | -12.340 | 44.938 | 1.00 10.03 |
| | 14442 | | ASP | 2164 | | -13.822 | 44.607 | 1.00 10.37 |
| MOTA | | CB | | 2164 | | -14.029 | 43.373 | 1.00 10.37 |
| ATOM | 14443 | CG | ASP | | | | | |
| ATOM | 14444 | | ASP | 2164 | | -13.141 | 43.044 | |
| ATOM | 14445 | | ASP | 2164 | | -15.107 | 42.745 | 1.00 14.94 |
| ATOM | 14446 | C | ASP | 2164 | | -12.250 | 46.260 | 1.00 12.25 |
| ATOM | 14447 | 0 | ASP | 2164 | | -11.971 | 47.313 | 1.00 11.28 |
| MOTA | 14448 | N | ILE | 2165 | | -12.500 | 46.212 | 1.00 13.30 |
| MOTA | 14449 | CA | ILE | 2165 | | -12.429 | 47.433 | 1.00 11.13 |
| MOTA | 14450 | CB | ILE | 2165 | | -12.815 | 47.165 | 1.00 10.95 |
| MOTA | 14451 | CG2 | | 2165 | | -12.571 | 48.418 | 1.00 12.50 |
| ATOM | 14452 | CG1 | | 2165 | | -14.287 | 46.734 | 1.00 9.88 |
| MOTA | 14453 | CD1 | | 2165 | | -15.294 | 47.819 | 1.00 13.15 |
| MOTA | 14454 | С | ILE | 2165 | | -11.024 | 48.041 | 1.00 11.12 |
| MOTA | 14455 | -O | ILE | 2165 | | -10.861 | 49.249 | 1.00 12.10 |
| ATOM | 14456 | N | ALA | 2166 | | -10.016 | 47.195 | 1.00 11.76 |
| ATOM | 14457 | CA | ALA | 2166 | 15.471 | -8.618 | 47.634 | 1.00 11.59 |
| MOTA | 14458 | CB | ALA | 2166 | 15.742 | -7.710 | 46.439 | 1.00 13.22 |
| MOTA | 14459 | С | ALA | 2166 | 14.154 | -8.214 | 48.303 | 1.00 13.49 |
| MOTA | 14460 | 0 | ALA | 2166 | 14.139 | 7.453 | 49.278 | 1.00 12.63 |
| MOTA | 14461 | N | TYR | 2167 | 13.056 | -8.704 | 47.738 | 1.00 12.03 |
| MOTA | 14462 | CA | TYR | 2167 | 11.710 | -8.448 | 48.230 | 1.00 12.41 |
| ATOM | 14463 | CB | TYR | 2167 | 10.711 | -9.189 | 47.334 | 1.00 13.48 |
| ATOM | 14464 | CG | TYR | 2167 | 9.281 | -9.135 | 47.805 | 1.00 12.75 |
| ATOM | 14465 | CD1 | TYR | 2167 | 8.555 | -7.946 | 47.742 | 1.00 15.28 |
| ATOM | 14466 | CE1 | TYR | 2167 | 7.228 | -7.895 | 48.153 | 1.00 14.62 |
| MOTA | 14467 | CD2 | TYR | 2167 | 8.645 | -10.276 | 48.299 | 1.00 13.65 |
| ATOM | 14468 | CE2 | TYR | 2167 | 7.316 | -10.233 | 48.715 | 1.00 13.81 |
| ATOM | 14469 | CZ | TYR | 2167 | 6.617 | -9.038 | 48.637 | 1.00 13.06 |
| ATOM | 14470 | ОН | TYR | 2167 | 5.303 | -8.988 | 49.050 | 1.00 15.51 |
| ATOM | 14471 | С | TYR | 2167 | 11.578 | -8.966 | 49.660 | 1.00 13.47 |
| ATOM | 14472 | . 0 | TYR | 2167 | 11.200 | -8.242 | 50.585 | 1.00 14.07 |
| MOTA | 14473 | N | HIS | 2168 | 11.902 | -10.241 | 49.824 | 1.00 13.89 |
| MOTA | 14474 | CA | HIS | 2168 | 11.823 | -10.890 | 51.120 | 1.00 13.79 |
| MOTA | 14475 | CB | HIS | 2168 | | -12.403 | 50.929 | 1.00 12.97 |
| ATOM | 14476 | CG | HIS | 2168 | 10.731 | -13.014 | 50.289 | 1.00 14.62 |
| ATOM | 14477 | | HIS | 2168 | | -13.400 | 49.012 | 1.00 13.57 |
| ATOM | 14478 | | HIS | 2168 | | -13.220 | 50.976 | 1.00 13.84 |
| ATOM | 14479 | | HIS | 2168 | | -13.706 | | 1.00 15.74 |
| ATOM | 14480 | | HIS | 2168 | | -13.825 | 48.954 | 1.00 11.68 |
| ATOM | 14481 | С | HIS | 2168 | | -10.356 | 52.104 | 1.00 14.35 |
| ATOM | 14482 | 0 | HIS | 2168 | 12.634 | -10.331 | 53.313 | 1.00 14.35 |
| ATOM | 14483 | N | THR | 2169 | 14.011 | -9.913 | 51.585 | 1.00 14.47 |
| ATOM | 14484 | CA | THR | 2169 | 15.068 | -9.369 | 52.428 | 1.00 14.38 |
| ATOM | 14485 | СВ | THR | 2169 | 16.367 | -9.150 | 51.611 | 1.00 15.28 |
| ATOM | 14486 | OG1 | | 2169 | | 10.425 | 51.308 | 1.00 12.29 |
| ATOM | 14487 | CG2 | THR | 2169 | 17.369 | -8.307 | 52.395 | 1.00 14.61 |
| ATOM | 14488 | C | THR | 2169 | 14.617 | -8.050 | 53.079 | 1.00 14.47 |
| ATOM | 14489 | ō | THR | 2169 | 14.784 | -7.857 | 54.288 | 1.00 14.08 |
| ATOM | 14490 | N | ALA | 2170 | 14.025 | -7.155 | 52.294 | 1.00 13.56 |
| ATOM | 14491 | CA | ALA | 2170 | 13.567 | -5.886 | 52.840 | 1.00 13.22 |
| ATOM | 14492 | CB | ALA | 2170 | 13.008 | -4.999 | 51.723 | 1.00 12.46 |
| ATOM | 14493 | C | ALA | 2170 | 12.498 | -6.141 | 53.905 | 1.00 15.28 |
| ATOM | 14494 | 0 | ALA | 2170 | 12.467 | | 54.946 | 1.00 13.20 |
| ATOM | 14495 | N | ALA | 2171 | 11.635 | -7.123 | 53.657 | 1.00 15.33 |
| ATOM | 14496 | CA | ALA | 2171 | 10.580 | -7.447 | 54.613 | 1.00 15.79 |
| ATOM | 14497 | CB | ALA | 2171 | 9.646 | -8.500 | 54.033 | 1.00 15.79 |
| ATOM | 14498 | С | ALA | 2171 | 11.163 | -7.932 | 55.936 | 1.00 15.33 |
| ATOM | 14499 | 0 | ALA | 2171 | 10.733 | -7.500 | 57.010 | 1.00 16.02 |
| ATOM | 14500 | N | VAL | 2171 | 12.146 | -8.824 | 55.868 | 1.00 16.63 |
| ATOM | 14501 | CA | VAL | 2172 | 12.771 | -9.341 | 57.085 | 1.00 16.03 |
| ATOM | 14501 | CB | VAL | 2172 | | -10.494 | 56.762 | 1.00 10.23 |
| ATOM | 14503 | | VAL | 2172 | | -10.434 | 57.979 | 1.00 17.31 |
| ATOM | 14504 | | VAL | 2172 | | -11.742 | 56.338 | 1.00 16.91 |
| | | | | | ,,,,, | , | | |

| ATOM | 14505 | С | VAL | 2172 | 13.484 | -8.213 | 57.831 | 1.00 16.90 |
|------|-------|-----|-----|-------------------|--------|---------|---------|------------|
| MOTA | 14506 | 0 | VAL | 2172 | 13.432 | -8.155 | 59.063 | 1.00 18.87 |
| ATOM | 14507 | N | ARG | 2173 | 14.138 | -7.321 | 57.089 | 1.00 16.84 |
| ATOM | 14508 | CA | ARG | 2173 | 14.860 | -6.195 | 57.689 | 1.00 17.87 |
| MOTA | 14509 | CB | ARG | 2173 | 15.594 | -5.380 | 56.613 | 1.00 18.06 |
| ATOM | 14510 | CG | ARG | 2173 | 16.334 | -4.149 | 57.156 | 1.00 17.82 |
| ATOM | 14511 | CD | ARG | 2173 | 17.239 | -4.512 | 58.340 | 1.00 19.45 |
| ATOM | 14512 | NE | ARG | 2173 | 18.482 | -5.163 | 57.929 | 1.00 18.22 |
| MOTA | 14513 | CZ | ARG | 2173 | 19.265 | -5.871 | 58.740 | 1.00 18.73 |
| ATOM | 14514 | NH1 | ARG | 2173 | 18.946 | -6.037 | 60.017 | 1.00 17.92 |
| ATOM | 14515 | NH2 | ARG | 2173 | 20.375 | -6.418 | 58.274 | 1.00 17.07 |
| ATOM | 14516 | С | ARG | 2173 | 13.915 | -5.283 | 58.467 | 1.00 19.95 |
| ATOM | 14517 | 0 | ARG | 2173 | 14.280 | -4.753 | 59.523 | 1.00 18.61 |
| MOTA | 14518 | N | ARG | 2174 | 12.707 | -5.089 | 57.945 | 1.00 18.95 |
| ATOM | 14519 | CA | ARG | 2174 | 11.722 | -4.260 | 58.638 | 1.00 20.06 |
| MOTA | 14520 | CB | ARG | 2174 | 10.477 | -4.041 | 57.774 | 1.00 18.51 |
| MOTA | 14521 | CG | ARG | 2174 | 10.726 | -3.306 | 56.483 | 1.00 20.20 |
| MOTA | 14522 | CD | ARG | 2174 | 9.422 | -2.876 | 55.813 | 1.00 22.84 |
| ATOM | 14523 | NE | ARG | 2174 | 9.707 | -2.195 | 54.558 | 1.00 24.12 |
| MOTA | 14524 | CZ | ARG | 2174 | 9.783 | -2.796 | 53.375 | 1.00 26.27 |
| MOTA | 14525 | NH1 | ARG | 2174 | 9.576 | -4.103 | 53.268 | 1.00 23.46 |
| MOTA | 14526 | NH2 | ARG | 2174 | 10.109 | -2.092 | 52.302 | 1.00 28.61 |
| ATOM | 14527 | С | ARG | 2174 | 11.319 | -4.976 | 59.916 | 1.00 19.12 |
| MOTA | 14528 | 0 | ARG | 2174 | 11.045 | -4.344 | 60.932 | 1.00 22.06 |
| MOTA | 14529 | N | GLY | 2175 | 11.289 | -6.304 | 59.863 | 1.00 18.76 |
| MOTA | 14530 | CA | GLY | 2175 | 10.910 | -7.080 | 61.034 | 1.00 19.18 |
| MOTA | 14531 | С | GLY | 2175 | 11.974 | -7.136 | 62.117 | 1.00 19.83 |
| ATOM | 14532 | 0 | GLY | 2175 | 11.662 | -7.173 | 63.311 | 1.00 19.15 |
| ATOM | 14533 | N | ALA | 2176 [°] | 13.235 | -7.126 | 61.695 | 1.00 17.37 |
| MOTA | 14534 | CA | ALA | 2176 | 14.365 | -7.203 | 62.619 | 1.00 19.31 |
| MOTA | 14535 | CB | ALA | 2176 | 14.875 | -8.644 | 62.690 | 1.00 20.30 |
| MOTA | 14536 | С | ALA | 2176 | 15.481 | -6.278 | 62.155 | 1.00 20.49 |
| MOTA | 14537 | 0 | ALA | 2176 | 16.462 | -6.728 | 61.560 | 1.00 20.07 |
| MOTA | 14538 | N | PRO | 2177 | 15.354 | -4.972 | 62.444 | 1.00 21.58 |
| MOTA | 14539 | CD | PRO | 2177 | 14.298 | -4.390 | 63.294 | 1.00 22.88 |
| ATOM | 14540 | CA | PRO | 2177 | 16.328 | -3.943 | 62.064 | 1.00 22.64 |
| ATOM | 14541 | CB | PRO | 2177 | 15.653 | -2.655 | 62.514 | 1.00 22.85 |
| MOTA | 14542 | CG | PRO | 2177 | 14.934 | -3.088 | 63.739 | 1.00 25.21 |
| ATOM | 14543 | С | PRO | 2177 | 17.734 | -4.080 | 62.631 | 1.00 22.77 |
| MOTA | 14544 | . 0 | PRO | 2177 | 18.663 | -3.437 | 62.139 | 1.00 23.87 |
| MOTA | 14545 | N | ASN | 2178 | 17.902 | -4.910 | 63.654 | 1.00 22.77 |
| ATOM | 14546 | CA | ASN | 2178 | 19.222 | -5.085 | 64.255 | 1.00 24.54 |
| ATOM | 14547 | CB | ASN | 2178 | 19.166 | -4.740 | 65.747 | 1.00 28.89 |
| MOTA | 14548 | CG | ASN | 2178 | 18.808 | -3.287 | 65.993 | 1.00 31.12 |
| MOTA | 14549 | OD1 | ASN | 2178 | 19.380 | -2.389 | -65.380 | 1.00 32.75 |
| ATOM | 14550 | ND2 | ASN | 2178 | 17.861 | -3.049 | 66.897 | 1.00 35.74 |
| ATOM | 14551 | ,C | ASN | 2178 | 19.814 | | 64.078 | 1.00 22.89 |
| MOTA | 14552 | 0 | ASN | 2178 | 20.908 | -6.771 | 64.573 | 1.00 21.60 |
| MOTA | 14553 | N | CYS | 2179 | 19.105 | -7.343 | 63.359 | 1.00 21.20 |
| MOTA | 14554 | CA | CYS | 2179 | 19.578 | -8.708 | 63.156 | 1.00 19.54 |
| MOTA | 14555 | CB | CYS | 2179 | 18.419 | -9.616 | 62.719 | 1.00 22.19 |
| MOTA | 14556 | SG | CYS | 2179 | 18.150 | -9.714 | | 1.00 21.61 |
| ATOM | 14557 | С | CYS | 2179 | 20.686 | -8.781 | 62.114 | 1.00 18.00 |
| ATOM | 14558 | 0 | CYS | 2179 | 20.898 | -7.845 | 61.336 | 1.00 16.56 |
| ATOM | 14559 | N | LEU | 2180 | 21.427 | -9.882 | 62.144 | 1.00 17.26 |
| ATOM | 14560 | CA | LEU | 2180 . | | -10.121 | 61.147 | 1.00 18.03 |
| ATOM | 14561 | CB | LEU | 2180 | | -11.046 | 61.684 | 1.00 18.50 |
| ATOM | 14562 | CG | LEU | 2180 | | -11.437 | 60.655 | 1.00 18.21 |
| ATOM | 14563 | | LEU | 2180 | | -10.206 | 60.115 | 1.00 19.75 |
| ATOM | 14564 | CD2 | LEU | 2180 | | -12.392 | 61.293 | 1.00 21.75 |
| ATOM | 14565 | C | LEU | 2180 | | -10.853 | 60.092 | 1.00 15.89 |
| ATOM | 14566 | 0 | LEU | 2180 | | -11.958 | 60.338 | 1.00 15.61 |
| ATOM | 14567 | N | LEU | 2181 | | -10.229 | 58.933 | 1.00 16.34 |
| ATOM | 14568 | CA | LEU | 2181 | | -10.802 | 57.865 | 1.00 15.32 |
| ATOM | 14569 | CB | LEU | 2181 | 19.730 | -9.734 | 57.308 | 1.00 14.91 |
| ATOM | 14570 | CG | LEU | 2181 | | -10.175 | 56.612 | 1.00 15.55 |
| ATOM | 14571 | | LEU | 2181 | 17.575 | -8.936 | 56.395 | 1.00 16.38 |
| ATOM | 14572 | | LEU | 2181 | | -10.863 | 55.293 | 1.00 20.67 |
| MOTA | 14573 | C | LEU | 2181 | | -11.382 | 56.727 | 1.00 13.75 |
| MOTA | 14574 | 0 | LEU | 2181 | | -10.657 | 56.053 | 1.00 14.71 |
| MOTA | 14575 | N | LEU | 2182 | | -12.690 | 56.525 | 1.00 13.90 |
| MOTA | 14576 | CA | LEU | 2182 | | -13.329 | 55.435 | 1.00 15.95 |
| ATOM | 14577 | CB | LEU | 2182 | | -14.660 | 55.875 | 1.00 15.67 |
| ATOM | 14578 | CG | LEU | 2182 | | -14.629 | 56.437 | 1.00 20.08 |
| MOTA | 14579 | | LEU | 2182 | | -13.819 | 57.715 | 1.00 19.21 |
| ATOM | 14580 | | LEU | 2182 | | -16.065 | 56.686 | 1.00 19.28 |
| MOTA | 14581 | С | LEU | 2182 | ∠⊥.⊥36 | -13.585 | 54.308 | 1.00 15.71 |

| | MOTA | 14582 | 0 | LEU | 2182 | 20.040 | -14.075 | 54.552 | 1.00 19.38 |
|---|--------------|----------------|----------|------------|--------------|--------|--------------------|------------------|--------------------------|
| | ATOM | 14583 | N | ALA | 2183 | 21.508 | -13.246 | 53.081 | 1.00 13.91 |
| | MOTA | 14584 | CA | ALA | 2183 | 20.614 | -13.486 | 51.962 | 1.00 14.60 |
| | MOTA | 14585 | CB | ALA | 2183 | 20.126 | -12.169 | 51.386 | 1.00 13.61 |
| | MOTA | 14586 | C | ALA | 2183 | | -14.305 | 50.893 | 1.00 14.00 |
| | MOTA | 14587 | 0 | ALA | 2183 | 22.471 | -14.049 | 50.538 | 1.00 11.35 |
| | MOTA | 14588 | N | ASP | 2184 | 20.609 | -15.309 | 50.388 | 1.00 14.08 |
| | MOTA | 14589 | CA | ASP | 2184 | 21.169 | -16.162 | 49.346 | 1.00 16.54 |
| | MOTA | 14590 | CB | ASP | 2184 | 20.341 | -17.439 | 49.180 | 1.00 16.86 |
| | MOTA | 14591 | CG | ASP | 2184 | 20.733 | -18.535 | 50.138 | 1.00 20.98 |
| | MOTA | 14592 | OD1 | ASP | 2184 - | | -18.459 | 50.747 | 1.00 22.21 |
| | MOTA | 14593 | | ASP | 2184 | | -19.496 | 50.255 | 1.00 20.02 |
| | MOTA | 14594 | C | ASP | 2184 | | -15.479 | 47.997 | 1.00 14.79 |
| | MOTA | 14595 | О | ASP | 2184 | | -14.678 | 47.694 | 1.00 15.78 |
| | MOTA | 14596 | N | LEU | 2185 | | -15.764 | 47.200 | 1.00 14.30 |
| | MOTA | 14597 | CA | LEU | 2185 | | -15.275 | 45.831 | 1.00 13.25 |
| | MOTA | 14598 | CB | LEU | 2185 | | -15.010 | 45.302 | 1.00 15.09 |
| | MOTA | 14599 | CG | LEU | 2185 | | -13.667 | 45.767 | 1.00 16.23 1.00 17.48 |
| | ATOM | 14600 | CD1 | LEU | 2185 | | -13.358 | 44.938 | 1.00 17.48 1.00 14.68 |
| | MOTA | 14601 | CD2 | LEU | 2185 | | -12.546 | 45.571 45.211 | 1.00 14.00 |
| | MOTA | 14602 | С | LEU LEU | 2185 2185 | | -16.538 -17.652 | 45.436 | 1.00 13.37 |
| | MOTA | 14603 14604 | O N | PRO | 2186 | | -16.391 | 44.456 | 1.00 13.10 |
| | ATOM ATOM | 14605 | CD | PRO | 2186 | | -15.118 | 44.188 | 1.00 15.09 |
| | ATOM | 14606 | CA | PRO | 2186 | | -17.516 | 43.817 | 1.00 14.43 |
| | ATOM | 14607 | CB | PRO | 2186 | | -16.910 | 43.396 | 1.00 15.40 |
| | ATOM | 14608 | CG | PRO | 2186 | | -15.483 | 43.085 | 1.00 15.67 |
| | ATOM | 14609 | C | PRO | 2186 | | -18.177 | 42.663 | 1.00 14.33 |
| | ATOM | 14610 | ō | PRO | 2186 | | -17.782 | 42.302 | 1.00 15.03 |
| | ATOM | 14611 | N | PHE | 2187 | | -19.197 | 42.100 | 1.00 13.69 |
| | ATOM | 14612 | CA | PHE | 2187 | | -19.951 | 40.977 | 1.00 12.48 |
| | ATOM | 14613 | СВ | PHE | 2187 | | -20.933 | 40.493 | 1.00 10.11 |
| | ATOM | 14614 | CG | PHE | 2187 | 19.660 | -21.528 | 39.131 | 1.00 13.16 |
| | MOTA | 14615 | CD1 | PHE | 2187 | 20.749 | -22.365 | 38.904 | 1.00 11.33 |
| | MOTA | 14616 | CD2 | PHE | 2187 | 18.751 | -21.300 | 38.088 | 1.00 12.80 |
| | MOTA | 14617 | CE1 | PHE | 2187 | 20.934 | -22.979 | 37.655 | 1.00 14.13 |
| | MOTA | 14618 | CE2 | PHE | 2187 | 18.914 | -21.899 | 36.837 | 1.00 12.25 |
| | MOTA | 14619 | CZ | PHE | 2187 | 20.005 | -22.739 | 36.619 | 1.00 13.80 |
| | MOTA | 14620 | С | PHE | 2187 | | -19.024 | 39.849 | 1.00 11.25 |
| | MOTA | 14621 | 0 | PHE | 2187 | | -18.098 | 39.452 | 1.00 11.41 |
| | MOTA | 14622 | N | MET | 2188 | | -19.282 | 39.358 | 1.00 12.61 |
| | MOTA | 14623 | CA | MET | 2188 | | -18.531 | 38.275 | 1.00 13.77 |
| | MOTA | 14624 | CB | MET | 2188 | | -18.862 | 36.943 | 1.00 13.96 |
| | MOTA | 14625 | CG | MET | 2188 | | -18.723 | 35.707 | 1.00 16.90 |
| | MOTA | 14626- | SD | MET | 2188 | | -19.853 | 35.851 | 1.00 12.86 |
| | MOTA | 14627 | CE | MET | 2188 | 23.813 | -21.357 | 35.069 | 1.00 19.25 |
| | ATOM | 14628 | C | MET | 2188 | | -17.015 | 38.519 | 1.00 14.59 1.00 16.18 |
| | MOTA | 14629 | 0 | MET | 2188 | | -16.226 -16.599 | 37.584 39.775 | 1.00 13.18 |
| | ATOM | 14630 | N | ALA | 2189 | 22.933 | -15.167 | 40.099 | 1.00 13.29 |
| | ATOM ATOM | 14631 14632 | CA CB | ALA ALA | 2189 2189 | 22.366 | -14.864 | 41.333 | 1.00 13.72 |
| | ATOM | 14633 | СВ | ALA | 2189 | | -14.747 | | 1.00 14.21 |
| | | | 0 | ALA | 2189 | | -13.580 | 40.633 | 1.00 15.89 |
| | ATOM ATOM | 14634 14635 | N | TYR | 2190 | | -15.708 | 40.278 | 1.00 12.28 |
| | ATOM | 14636 | CA | TYR | 2190 | | -15.433 | 40.483 | 1.00 13.07 |
| | ATOM | 14637 | CB | TYR | 2190 | | -15.714 | 41.946 | 1.00 12.91 |
| | ATOM | 14638 | CG | TYR | 2190 | | -17.035 | 42.515 | 1.00 11.62 |
| | ATOM | 14639 | CD1 | TYR | 2190 | | -18.156 | 42.554 | 1.00 11.92 |
| • | ATOM | 14640 | CE1 | TYR | 2190 | | -19.366 | 43.090 | 1.00 12.64 |
| | ATOM | 14641 | CD2 | TYR | 2190 | | -17.158 | 43.027 | 1.00 14.06 |
| | MOTA | 14642 | CE2 | TYR | 2190 | 24.944 | -18.360 | 43.563 | 1.00 13.68 |
| | MOTA | 14643 | CZ | TYR | 2190 | 25.793 | -19.461 | 43.593 | 1.00 14.72 |
| | MOTA | 14644 | ОН | TYR | 2190 | | -20.652 | 44.128 | 1.00 15.24 |
| | MOTA | 14645 | С | TYR | 2190 | | -16.262 | 39.515 | 1.00 14.64 |
| | MOTA | 14646 | 0 | TYR | 2190 | 28.681 | -16.822 | 39.887 | 1.00 14.18 |
| | ATOM | 14647 | N | ALA | 2191 | | -16.316 | 38.267 | 1.00 13.79 |
| | ATOM | 14648 | CA | ALA | 2191 | | -17.062 | 37.194 | 1.00 14.38 |
| | MOTA | 14649 | CB | ALA | 2191 | | -17.077 | 35.976 | 1.00 13.74 |
| | MOTA | 14650 | C | ALA | 2191 | | -16.503 | 36.808 | 1.00 13.17 |
| | MOTA | 14651 | 0 | ALA | 2191 | | -17.240 | 36.331 | 1.00 12.13 |
| | ATOM | 14652 | N | THR | 2192 | 29.382 | -15.198 | 36.998 | 1.00 12.89 |
| | MOTA | 14653 | CA | THR | 2192 | | -14.500 | 36.705 | 1.00 14.63 |
| | MOTA | 14654 | CB | THR | 2192 | | -13.704 | 35.386 | 1.00 15.14 1.00 13.87 |
| | ATOM | 14655 | OG1 | THR | 2192 | | -12.583 | 35.546 | 1.00 13.87 |
| | ATOM | 14656 | CG2 | THR | 2192 | | -14.589 -13.495 | 34.254 37.835 | 1.00 15.22 |
| | MOTA MOTA | 14657 14658 | C O | THR THR | 2192 2192 | | -13.495 | 38.517 | 1.00 15.41 |
| | 111011 | 14070 | 0 | 1111 | 2172 | 27.013 | 10.120 | 50.51, | |
| | | | | | | | | | |

| ATOM | 14659 | N | PRO | 2193 | 32.073 | -13.042 | 38.053 | 1.00 16.19 |
|--------------|----------------|-----------|------------|--------------|------------------|--------------------|------------------|--------------------------|
| ATOM | 14660 | CD | PRO | 2193 | 33.343 | -13.538 | 37.490 | 1.00 16.85 |
| MOTA | 14661 | CA | PRO | 2193 | 32.315 | -12.073 | 39.124 | 1.00 16.55 |
| MOTA | 14662 | CB | PRO | 2193 | 33.803 | -11.792 | 38.992 | 1.00 18.64 |
| MOTA | 14663 | CG | PRO | 2193 | 34.343 | -13.133 | 38.552 | 1.00 17.11 |
| ATOM | 14664 | C | PRO | 2193 | 31.465 | -10.824 | 38.937 | 1.00 15.31 |
| ATOM | 14665 | 0 | PRO | 2193 | 30.831 | -10.354 | 39.876 | 1.00 15.59 |
| ATOM | 14666 | N | GLU | 2194 | 31.454 | -10.296 | 37.718 | 1.00 16.75 |
| MOTA | 14667 | CA | GLU | 2194 | 30.687 | -9.098 -8.711 | 37.419 35.948 | 1.00 17.91 1.00 23.31 |
| ATOM ATOM | 14668 14669 | CB CG | GLU GLU | 2194 2194 | 30.858 32.215 | -8.092 | 35.630 | 1.00 30.85 |
| ATOM | 14670 | CD | GLU | 2194 | 32.409 | -7.831 | 34.149 | 1.00 35.36 |
| ATOM | 14671 | OE1 | | 2194 | 31.524 | -7.192 | 33.537 | 1.00 39.04 |
| ATOM | 14672 | OE2 | GLU | 2194 | 33.450 | -8.260 | 33.598 | 1.00 39.02 |
| ATOM | 14673 | С | GLU | 2194 | 29.206 | -9.245 | 37.757 | 1.00 17.81 |
| MOTA | 14674 | 0 | GLU | 2194 | 28.602 | -8.322 | 38.304 | 1.00 17.37 |
| ATOM | 14675 | N | GLN | 2195 | 28.612 | -10.390 | 37.435 | 1.00 15.20 |
| MOTA | 14676 | CA | GLN | 2195 | 27.199 | -10.586 | 37.744 | 1.00 16.01 |
| ATOM | 14677 | CB | GLN | 2195 | 26.642 | -11.799 | 36.994 | 1.00 17.15 |
| ATOM | 14678 | CG | GLN | 2195 | 26.551 | -11.574 | 35.488 | 1.00 21.26 |
| ATOM | 14679 | CD | GLN | 2195 | 26.048 | -12.795 -13.304 | 34.750 35.038 | 1.00 25.19 1.00 25.51 |
| ATOM ATOM | 14680 14681 | OE1 | GLN GLN | 2195 2195 | | -13.304 | 33.787 | 1.00 28.35 |
| ATOM | 14682 | C | GLN | 2195 | 27.006 | -10.756 | 39.248 | 1.00 14.45 |
| ATOM | 14683 | 0 | GLN | 2195 | 26.010 | -10.300 | 39.798 | 1.00 14.86 |
| ATOM | 14684 | N | ALA | 2196 | 27.966 | -11.407 | 39.899 | 1.00 12.21 |
| ATOM | 14685 | CA | ALA | 2196 | 27.908 | -11.620 | 41.329 | 1.00 12.40 |
| ATOM | 14686 | CB | ALA | 2196 | 29.105 | -12.455 | 41.795 | 1.00 13.23 |
| ATOM | 14687 | С | ALA | 2196 | 27.898 | -10.272 | 42.047 | 1.00 11.64 |
| ATOM | 14688 | 0 | ALA | 2196 | 27.146 | -10.072 | 43.010 | 1.00 11.62 |
| ATOM | 14689 | N | PHE | 2197 | 28.727 | -9.346 | 41.571 | 1.00 11.56 |
| MOTA | 14690 | CA | PHE | 2197 | 28.809 | -8.007 | 42.164 | 1.00 13.89 |
| ATOM | 14691 | CB | PHE | 2197 | 29.858 | -7.146 | 41.442 | 1.00 13.21 |
| MOTA | 14692 | CG CD1 | PHE | 2197 | 31.236 | -7.743 -8.576 | 41.414 42.432 | 1.00 12.74 1.00 13.16 |
| ATOM ATOM | 14693 14694 | | PHE PHE | 2197 2197 | 31.673 32.106 | -7.448 | 40.368 | 1.00 13.10 |
| ATOM | 14695 | CE1 | | 2197 | 32.962 | -9.119 | 42.413 | 1.00 17.01 |
| ATOM | 14696 | | PHE | 2197 | 33.397 | -7.981 | 40.332 | 1.00 15.05 |
| ATOM | 14697 | CZ | PHE | 2197 | 33.819 | -8.815 | 41.355 | 1.00 15.53 |
| MOTA | 14698 | С | PHE | 2197 | 27.469 | -7.282 | 42.071 | 1.00 15.38 |
| MOTA | 14699 | 0 | PHE | 2197 | 26.976 | -6.713 | 43.047 | 1.00 15.31 |
| ATOM | 14700 | N | GLU | 2198 | 26.900 | -7.296 | 40.874 | 1.00 16.38 |
| MOTA | 14701 | CA | GLU | 2198 | 25.636 | -6.629 | 40.619 | 1.00 18.38 |
| MOTA | 14702 | CB | GLU | 2198 | 25.286 | -6.745 | 39.134 | 1.00 21.89 |
| MOTA | 14703 | CG | GLU | 2198 | 24.046 | -5.985 | 38.698 | 1.00 28.47 |
| MOTA | 14704 14705 | CD OF1 | GLU GLU | 2198 2198 | 24.133 25.253 | -4.486 -3.974 | 38.975 39.213 | 1.00 31.20 1.00 31.05 |
| ATOM ATOM | 14706 | OE2 | | 2198 | 23.233 | -3.823 | 38.939 | 1.00 33.83 |
| ATOM | 14707 | C | GLU | 2198 | 24.502 | -7.198 | 41.463 | 1.00 16.31 |
| ATOM | 14708 | ō | GLU | 2198 | 23.748 | -6.451 | 42.088 | 1.00 15.63 |
| ATOM | 14709 | N | ASN | 2199 | 24.390 | -8.520 | 41.488 | 1.00 14.90 |
| ATOM | 14710 | CA | ASN | 2199 | 23.331 | -9.173 | 42.234 | 1.00 15.15 |
| MOTA | 14711 | CB | ASN | 2199 | 23.176 | -10.619 | 41.748 | 1.00 14.55 |
| MOTA | 14712 | CG | ASN | 2199 | 22.703 | -10.687 | 40.306 | 1.00 14.12 |
| ATOM | 14713 | | ASN | 2199 | 21.887 | -9.869 | 39.880 | 1.00 13.06 |
| ATOM | 14714 | | ASN | 2199 | 23.196 | -11.666 | 39.551 43.737 | 1.00 16.16 1.00 13.30 |
| ATOM ATOM | 14715 14716 | С 0 | ASN ASN | 2199 2199 | 23.537 22.576 | -9.112 -8.971 | 44.494 | 1.00 13.30 |
| MOTA | 14717 | N · | ALA | 2200 | 24.790 | -9.200 | 44.170 | 1.00 13.38 |
| ATOM | 14718 | CA | ALA | 2200 | 25.106 | -9.121 | 45.596 | 1.00 14.01 |
| ATOM | 14719 | CB | ALA | 2200 | 26.601 | -9.377 | 45.819 | 1.00 14.48 |
| MOTA | 14720 | С | ALA | 2200 | 24.738 | -7.720 | 46.092 | 1.00 12.03 |
| ATOM | 14721 | 0 | ALA | 2200 | 24.204 | -7.558 | 47.189 | 1.00 13.32 |
| MOTA | 14722 | N | ALA | 2201 | 25.022 | -6.713 | 45.271 | 1.00 13.67 |
| MOTA | 14723 | CA | ALA | 2201 | 24.716 | -5.335 | 45.625 | 1.00 13.13 |
| ATOM | 14724 | СВ | ALA | 2201 | 25.285 | -4.370 | 44.573 | 1.00 13.81 |
| ATOM · | 14725 | C | ALA | 2201 | 23.206 | -5.132 | 45.751 | 1.00 13.16 |
| ATOM | 14726 | O | ALA | 2201 | 22.736 | -4.435 -5.743 | 46.645 44.853 | 1.00 15.03 1.00 13.60 |
| MOTA | 14727 | N | THR | 2202 2202 | 22.446 20.999 | -5.743 -5.613 | 44.853 | 1.00 13.60 |
| ATOM ATOM | 14728 14729 | CA CB | THR THR | 2202 | 20.353 | -6.445 | 43.798 | 1.00 10.38 |
| ATOM | 14730 | | THR | 2202 | 20.822 | -5.973 | 42.537 | 1.00 10.36 |
| ATOM | 14731 | CG2 | | 2202 | 18.836 | -6.331 | 43.848 | 1.00 11.71 |
| MOTA | 14732 | c | THR | 2202 | 20.446 | -6.068 | 46.244 | 1.00 11.76 |
| MOTA | 14733 | 0 | THR | 2202 | 19.665 | -5.361 | 46.896 | 1.00 12.13 |
| MOTA | 14734 | N | VAL | 2203 | 20.867 | -7.252 | 46.658 | 1.00 11.71 |
| MOTA | 14735 | CA | VAL | 2203 | 20.431 | -7.835 | 47.908 | 1.00 14.15 |

| MOTA | 14736 | CB | VAL | 2203 | 20.883 | -9.303 | 47.970 | 1.00 17.90 |
|------|-------|-----|-----|------|----------|---------|--------|------------|
| MOTA | 14737 | CG1 | VAL | 2203 | 20.327 | -9.969 | 49.200 | 1.00 22.76 |
| ATOM | 14738 | CG2 | | 2203 | 20.393 | -10.031 | 46.713 | 1.00 21.66 |
| ATOM | 14739 | C | VAL | 2203 | 20.953 | -7.062 | 49.116 | 1.00 13.49 |
| | 14740 | ō | VAL | 2203 | 20.251 | -6.904 | 50.122 | 1.00 11.71 |
| ATOM | 14741 | N | MET | 2204 | 22.182 | -6.570 | 49.026 | 1.00 12.79 |
| MOTA | | | | | 22.743 | -5.798 | 50.136 | 1.00 15.57 |
| MOTA | 14742 | CA | MET | 2204 | | | 49.875 | |
| ATOM | 14743 | CB | MET | 2204 | 24.224 | -5.501 | | 1.00 16.63 |
| MOTA | 14744 | CG | MET | 2204 | 25.104 | -6.724 | 49.887 | 1.00 18.75 |
| MOTA | 14745 | SD | MET | 2204 | 25.263 | -7.508 | 51.497 | 1.00 19.13 |
| ATOM | 14746 | CE | MET | 2204 | 26.337 | -6.307 | 52.339 | 1.00 18.60 |
| ATOM | 14747 | C | MET | 2204 | 21.963 | -4.497 | 50.308 | 1.00 14.20 |
| ATOM | 14748 | 0 | MET | 2204 | 21.556 | -4.147 | 51.421 | 1.00 13.48 |
| MOTA | 14749 | N | ARG | 2205 | 21.739 | -3.785 | 49.208 | 1.00 13.14 |
| ATOM | 14750 | CA | ARG | 2205 | 20.995 | -2.527 | 49.284 | 1.00 13.16 |
| ATOM | 14751 | СВ | ARG | 2205 | 20.887 | -1.887 | 47.898 | 1.00 13.73 |
| | 14752 | CG | ARG | 2205 | 22.229 | -1.512 | 47.283 | 1.00 15.34 |
| MOTA | | | | | 22.044 | -0.529 | 46.141 | 1.00 14.72 |
| MOTA | 14753 | CD | ARG | 2205 | | | | |
| MOTA | 14754 | NE | ARG | 2205 | 23.263 | -0.355 | 45.349 | 1.00 16.85 |
| MOTA | 14755 | cz | ARG | 2205 | 23.591 | -1.101 | 44.299 | 1.00 15.47 |
| ATOM | 14756 | NH1 | ARG | 2205 | 22.791 | -2.083 | 43.900 | 1.00 16.64 |
| ATOM | 14757 | NH2 | ARG | 2205 | 24.717 | -0.857 | 43.642 | 1.00 16.81 |
| MOTA | 14758 | С | ARG | 2205 | 19.601 | -2.780 | 49.859 | 1.00 15.15 |
| ATOM | 14759 | 0 | ARG | 2205 | 19.033 | -1.919 | 50.530 | 1.00 13.24 |
| ATOM | 14760 | N | ALA | 2206 | 19.071 | -3.975 | 49.602 | 1.00 13.63 |
| ATOM | 14761 | CA | ALA | 2206 | 17.750 | -4.366 | 50.090 | 1.00 14.83 |
| MOTA | 14762 | CB | ALA | 2206 | 17.292 | -5.649 | 49.393 | 1.00 14.81 |
| | | | ALA | 2206 | 17.717 | -4.559 | 51.609 | 1.00 15.51 |
| MOTA | 14763 | C | | | | | | 1.00 15.01 |
| ATOM | 14764 | 0 | ALA | 2206 | 16.645 | -4.607 | 52.209 | |
| MOTA | 14765 | N | GLY | 2207 | 18.888 | -4.689 | 52.226 | 1.00 14.53 |
| MOTA | 14766 | CA | GLY | 2207 | 18.933 | -4.854 | 53.666 | 1.00 14.24 |
| MOTA | 14767 | С | GLY | 2207 | 19.806 | -5.969 | 54.210 | 1.00 14.79 |
| MOTA | 14768 | О | GLY | 2207 | 19.965 | -6.098 | 55.430 | 1.00 13.55 |
| MOTA | 14769 | N | ALA | 2208 | 20.384 | -6.782 | 53.330 | 1.00 13.05 |
| MOTA | 14770 | CA | ALA | 2208 | . 21.235 | -7.878 | 53.790 | 1.00 13.56 |
| ATOM | 14771 | CB | ALA | 2208 | 21.478 | -8.860 | 52.650 | 1.00 14.49 |
| АТОМ | 14772 | С | ALA | 2208 | 22.568 | -7.351 | 54.310 | 1.00 13.56 |
| ATOM | 14773 | o | ALA | 2208 | 22.982 | -6.257 | 53.946 | 1.00 14.11 |
| | 14774 | N | ASN | 2209 | 23.216 | -8.112 | 55.187 | 1.00 14.56 |
| ATOM | | | | | | | 55.720 | 1.00 16.30 |
| ATOM | 14775 | CA | ASN | 2209 | 24.526 | -7.715 | | |
| MOTA | 14776 | CB | ASN | 2209 | 24.596 | -7.881 | 57.236 | 1.00 17.22 |
| MOTA | 14777 | CG | ASN | 2209 | 23.534 | -7.107 | 57.964 | 1.00 15.22 |
| ATOM | 14778 | | ASN | 2209 | 23.458 | -5.884 | 57.868 | 1.00 20.45 |
| MOTA | 14779 | ND2 | ASN | 2209 | 22.707 | -7.821 | 58.711 | 1.00 13.67 |
| MOTA | 14780 | С | ASN | 2209 | 25.579 | -8.641 | 55.139 | 1.00 16.35 |
| ATOM | 14781 | 0 | ASN | 2209 | 26.776 | -8.360 | 55.194 | 1.00 16.50 |
| ATOM | 14782 | N | MET | 2210 | 25.113 | -9.755 | 54.594 | 1.00 16.82 |
| ATOM | 14783 | CA | MET | 2210 | 25.996 | -10.772 | 54.051 | 1.00 16.51 |
| ATOM | 14784 | CB | MET | 2210 | 26.474 | -11.661 | 55.197 | 1.00 18.41 |
| ATOM | 14785 | CG | MET | 2210 | 27.305 | -12.865 | 54.798 | 1.00 19.82 |
| | | | MET | 2210 | | -13.789 | 56.264 | 1.00 21.89 |
| MOTA | 14786 | SD | | | | | | |
| MOTA | 14787 | CE | MET | 2210 | | -13.207 | 56.418 | 1.00 21.07 |
| ATOM | 14788 | С | MET | 2210 | | -11.605 | 53.015 | 1.00 16.91 |
| MOTA | 14789 | 0 | MET | 2210 | | -11.784 | 53.100 | 1.00 14.74 |
| MOTA | 14790 | N | VAL | 2211 | 26.009 | -12.110 | 52.041 | 1.00 15.70 |
| MOTA | 14791 | CA | VAL | 2211 | 25.444 | -12.926 | 50.978 | 1.00 16.74 |
| MOTA | 14792 | CB | VAL | 2211 | 25.795 | -12.306 | 49.613 | 1.00 19.57 |
| MOTA | 14793 | CG1 | VAL | 2211 | 25.664 | -13.330 | 48.525 | 1.00 23.64 |
| MOTA | 14794 | CG2 | VAL | 2211 | 24.890 | -11.110 | 49.342 | 1.00 18.37 |
| ATOM | 14795 | C | VAL | 2211 | 25.982 | -14.356 | 51.052 | 1.00 17.23 |
| ATOM | 14796 | ō | VAL | 2211 | 27.151 | -14.570 | 51.388 | 1.00 17.13 |
| ATOM | 14797 | N | LYS | 2212 | 25.130 | -15.334 | 50.757 | 1.00 18.13 |
| | | | LYS | 2212 | 25.558 | -16.726 | 50.767 | 1.00 17.96 |
| MOTA | 14798 | CA | | | | | | |
| ATOM | 14799 | CB | LYS | 2212 | | -17.582 | 51.669 | 1.00 17.25 |
| MOTA | 14800 | CG | LYS | 2212 | 25.056 | -19.051 | 51.721 | 1.00 17.85 |
| MOTA | 14801 | CD | LYS | 2212 | 24.563 | -19.773 | 52.981 | 1.00 19.98 |
| ATOM | 14802 | CE | LYS | 2212 | 23.056 | -19.981 | 52.972 | 1.00 20.44 |
| ATOM | 14803 | NZ | LYS | 2212 | 22.617 | -20.726 | 51.751 | 1.00 19.76 |
| MOTA | 14804 | С | LYS | 2212 | 25.527 | -17.254 | 49.339 | 1.00 19.04 |
| MOTA | 14805 | 0 | LYS | 2212 | 24.612 | -16.947 | 48.568 | 1.00 18.54 |
| ATOM | 14806 | N | ILE | 2213 | 26.548 | -18.028 | 48.983 | 1.00 17.52 |
| ATOM | 14807 | CA | ILE | 2213 | 26.643 | -18.610 | 47.650 | 1.00 17.09 |
| ATOM | 14808 | CB | ILE | 2213 | 27.620 | -17.808 | 46.749 | 1.00 17.18 |
| ATOM | 14809 | CG2 | | 2213 | | -16.453 | 46.418 | 1.00 17.10 |
| | | | | | 28.972 | -17.636 | 47.447 | 1.00 19.73 |
| MOTA | 14810 | CG1 | | 2213 | | | | |
| ATOM | 14811 | CD1 | | 2213 | 29.984 | -16.858 | 46.638 | 1.00 18.91 |
| MOTA | 14812 | С | ILE | 2213 | ∠/.⊥⊥3 | -20.053 | 47.763 | 1.00 17.08 |

| ATOM | 14813 | 0 | ILE | 2213 | | 27.899 | -20.384 | 48.648 | 1.00 17.01 |
|------|-------|-----------|-------|------|---|--------|---------|--------|------------|
| ATOM | 14814 | N | GLU | 2214 | | | -20.908 | 46.868 | 1.00 17.34 |
| ATOM | 14815 | CA | GLU | 2214 | | | -22.331 | 46.885 | 1.00 18.18 |
| ATOM | 14816 | CB | GLU | 2214 | | | -23.170 | 46.518 | 1.00 19.12 |
| ATOM | 14817 | CG | GLU | 2214 | | | -22.784 | 47.239 | 1.00 20.19 |
| | | | GLU | 2214 | | | -23.676 | 46.855 | 1.00 23.23 |
| ATOM | 14818 | CD OD1 | | | | | | | |
| ATOM | 14819 | | GLU | 2214 | | | -24.392 | 45.835 | 1.00 22.32 |
| ATOM | 14820 | | GLU | 2214 | | | -23.657 | 47.563 | 1.00 22.19 |
| ATOM | 14821 | С | GLU | 2214 | | | -22.665 | 45.913 | 1.00 18.52 |
| ATOM | 14822 | 0 | GLU | 2214 | | | -22.200 | 44.775 | 1.00 17.83 |
| MOTA | 14823 | N | GLY | 2215 | | 29.048 | -23.467 | 46.361 | 1.00 19.25 |
| ATOM | 14824 | CA | GLY | 2215 | | 30.148 | -23.837 | 45.484 | 1.00 21.18 |
| ATOM | 14825 | С | GLY | 2215 | | 31.491 | -23.915 | 46.182 | 1.00 21.73 |
| ATOM | 14826 | 0 | GLY | 2215 | | 31.679 | -23.332 | 47.249 | 1.00 20.66 |
| ATOM | 14827 | N | GLY | 2216 | | | -24.629 | 45.575 | 1.00 22.21 |
| ATOM | 14828 | CA | GLY | 2216 | | | -24.765 | 46.176 | 1.00 21.89 |
| MOTA | 14829 | C | GLY | 2216 | | | -23.888 | 45.590 | 1.00 21.57 |
| ATOM | 14830 | ō | GLY | 2216 | | | -22.676 | 45.445 | 1.00 22.59 |
| ATOM | 14831 | N | GLU | 2217 | | | -24.524 | 45.266 | 1.00 22.40 |
| | 14832 | | GLU | 2217 | | | -23.869 | 44.701 | 1.00 22.40 |
| ATOM | | CA | | | | | -24.934 | | 1.00 25.30 |
| ATOM | 14833 | CB | GLU | 2217 | | | | 44.188 | |
| MOTA | 14834 | CG | GLU | 2217 | | | -25.430 | 45.213 | 1.00 34.27 |
| ATOM | 14835 | CD | GLU | 2217 | | | -24.431 | 45.458 | 1.00 37.56 |
| ATOM | 14836 | | GLU | 2217 | | | -23.296 | 45.880 | 1.00 41.29 |
| ATOM | 14837 | | GLU | 2217 | | | -24.777 | 45.223 | 1.00 40.20 |
| ATOM | 14838 | С | GLU | 2217 | | 36.881 | -22.869 | 43.584 | 1.00 20.77 |
| MOTA | 14839 | 0 | GLU | 2217 | | 37.519 | -21.817 | 43.531 | 1.00 19.61 |
| ATOM | 14840 | N | TRP | 2218 | | 35.950 | -23.185 | 42.690 | 1.00 19.83 |
| MOTA | 14841 | CA | TRP . | 2218 | ` | 35.678 | -22.291 | 41.576 | 1.00 18.55 |
| ATOM | 14842 | CB | TRP | 2218 | | 34.673 | -22.922 | 40.603 | 1.00 20.02 |
| ATOM | 14843 | CG | TRP | 2218 | | | -22.946 | 41.065 | 1.00 18.78 |
| ATOM | 14844 | CD2 | | 2218 | | | -22.023 | 40.687 | 1.00 17.40 |
| ATOM | 14845 | CE2 | TRP | 2218 | | | -22.440 | 41.318 | 1.00 16.35 |
| MOTA | 14846 | CE3 | TRP | 2218 | | | -20.881 | 39.875 | 1.00 15.52 |
| MOTA | 14847 | | TRP | 2218 | | | -23.860 | 41.889 | 1.00 19.14 |
| | | | | | | | -23.566 | | 1.00 19.14 |
| MOTA | 14848 | NE1 | | 2218 | | | | 42.044 | |
| MOTA | 14849 | CZ2 | TRP | 2218 | | | -21.753 | 41.161 | 1.00 17.53 |
| MOTA | 14850 | CZ3 | | 2218 | | | -20.199 | 39.719 | 1.00 17.03 |
| MOTA | 14851 | CH2 | | 2218 | | | -20.640 | 40.362 | 1.00 15.23 |
| ATOM | 14852 | С | TRP | 2218 | | | -20.906 | 42.006 | 1.00 17.22 |
| MOTA | 14853 | 0 | TRP | 2218 | | | -19.950 | 41.237 | 1.00 17.68 |
| ATOM | 14854 | N | LEU | 2219 | | 34.703 | -20.792 | 43.233 | 1.00 17.71 |
| ATOM | 14855 | CA | LEU | 2219 | • | 34.213 | -19.509 | 43.751 | 1.00 18.36 |
| MOTA | 14856 | CB | LEU | 2219 | | 33.130 | -19.746 | 44.809 | 1.00 18.12 |
| MOTA | 14857 | CG | LEU | 2219 | | 31.749 | -20.160 | 44.306 | 1.00 21.23 |
| ATOM | 14858 | CD1 | LEU | 2219 | | 30.838 | -20.464 | 45.498 | 1.00 21.25 |
| ATOM | 14859 | CD2 | | 2219 | | 31.158 | -19.035 | 43.455 | 1.00 19.14 |
| ATOM | 14860 | С | LEU | 2219 | | | -18.616 | 44.350 | 1.00 19.10 |
| ATOM | 14861 | ō | LEU | 2219 | | | -17.432 | 44.601 | 1.00 16.47 |
| ATOM | 14862 | N | VAL | 2220 | | | -19.178 | 44.577 | 1.00 18.67 |
| ATOM | 14863 | CA | VAL | 2220 | | | -18.417 | 45.162 | 1.00 19.82 |
| ATOM | 14864 | CB | | 2220 | | | -19.139 | | 1.00 10.02 |
| | | | | 2220 | | | | | |
| ATOM | 14865 | | VAL | | | | -18.231 | 45.324 | 1.00 21.55 |
| ATOM | 14866 | | VAL | 2220 | | | -20.415 | 45.742 | 1.00 22.40 |
| ATOM | 14867 | C | VAL | 2220 | | | -16.976 | 44.663 | 1.00 18.36 |
| MOTA | 14868 | 0 | VAL | 2220 | | | -16.045 | 45.457 | 1.00 19.22 |
| ATOM | 14869 | N | GLU | 2221 | | | -16.797 | 43.353 | 1.00 17.93 |
| ATOM | 14870 | CA | GLU | 2221 | | | -15.462 | 42.790 | 1.00 18.36 |
| MOTA | 14871 | CB | GLU | 2221 | | 38.208 | -15.543 | 41.281 | 1.00 20.61 |
| MOTA | 14872 | CG | GLU | 2221 | | 38.200 | -14.198 | 40.587 | 1.00 26.76 |
| ATOM | 14873 | CD | GLU | 2221 | | 38.529 | -14.303 | 39.113 | 1.00 30.40 |
| ATOM | 14874 | | GLU | 2221 | | | -15.014 | 38.385 | 1.00 30.39 |
| ATOM | 14875 | OE2 | GLU | 2221 | | 39.517 | -13.673 | 38.687 | 1.00 33.96 |
| ATOM | 14876 | С | GLU | 2221 | | | -14.567 | 43.091 | 1.00 18.56 |
| ATOM | 14877 | ō | GLU | | | | -13.395 | 43.436 | 1.00 16.57 |
| ATOM | 14878 | N | THR | 2222 | | | -15.126 | 42.946 | 1.00 17.43 |
| ATOM | 14879 | CA | THR | 2222 | | | -14.381 | 43.197 | 1.00 17.79 |
| MOTA | 14880 | CB | THR | | | | -15.243 | 42.872 | 1.00 17.79 |
| | | | | 2222 | | | | | |
| ATOM | 14881 | OG1 | | 2222 | | | -15.576 | 41.480 | 1.00 19.38 |
| ATOM | 14882 | CG2 | | 2222 | | | -14.485 | 43.188 | 1.00 19.18 |
| ATOM | 14883 | C | THR | 2222 | | | -13.895 | 44.645 | 1.00 16.86 |
| ATOM | 14884 | 0 | THR | 2222 | | | -12.741 | 44.904 | 1.00 15.36 |
| MOTA | 14885 | N | VAL | 2223 | | | -14.767 | 45.586 | 1.00 17.57 |
| ATOM | 14886 | CA | VAL | 2223 | | | -14.412 | 47.003 | 1.00 17.48 |
| ATOM | 14887 | CB | VAL | 2223 | | | -15.631 | 47.898 | 1.00 18.55 |
| MOTA | 14888 | | VAL | 2223 | | | -15.211 | 49.373 | 1.00 20.37 |
| ATOM | 14889 | CG2 | VAL | 2223 | | 33.932 | -16.721 | 47.652 | 1.00 16.46 |
| | | | | | | | | | |

| ATOM | 14890 | С | VAL | 2223 | 35.666 | -13.320 | 47.329 | 1.00 19.79 |
|------|-------|-----|------|-------|--------|---------|--------|------------|
| ATOM | 14891 | 0 | VAL | 2223 | 35.352 | -12.349 | 48.024 | 1.00 17.16 |
| ATOM | 14892 | N | GLN | 2224 | 36.885 | -13.489 | 46.827 | 1.00 18.72 |
| ATOM | 14893 | CA | GLN | 2224 | 37.940 | -12.515 | 47.065 | 1.00 21.39 |
| ATOM | 14894 | CB | GLN | 2224 | 39.233 | -12.925 | 46.346 | 1.00 24.26 |
| ATOM | 14895 | CG | GLN | 2224 | 39.725 | -14.335 | 46.648 | 1.00 29.53 |
| MOTA | 14896 | CD | GLN | 2224 | 41.050 | -14.655 | 45.953 | 1.00 33.18 |
| ATOM | 14897 | | GLN | 2224 | 41.196 | -14.464 | 44.738 | 1.00 33.20 |
| ATOM | 14898 | | GLN | 2224 | 42.018 | -15.150 | 46.722 | 1.00 32.66 |
| ATOM | 14899 | С | GLN | 2224 | 37.502 | -11.148 | 46.554 | 1.00 19.64 |
| ATOM | 14900 | 0 | GLN | 2224 | 37.628 | -10.149 | 47.253 | 1.00 19.34 |
| ATOM | 14901 | N | MET | 2225 | | -11.108 | 45.335 | 1.00 19.03 |
| ATOM | 14902 | CA | MET | 2225 | 36.552 | -9.846 | 44.744 | 1.00 18.40 |
| ATOM | 14903 | СВ | MET | 2225 | | -10.026 | 43.249 | 1.00 18.27 |
| ATOM | 14904 | CG | MET | 2225 | 37.591 | | 42.483 | 1.00 22.00 |
| ATOM | 14905 | SD | MET | 2225 | 37.353 | -10.429 | 40.706 | 1.00 21.95 |
| ATOM | 14906 | CE | MET | 2225 | 37.447 | -8.712 | 40.259 | 1.00 20.84 |
| ATOM | 14907 | С | MET | 2225 | 35.334 | -9.226 | 45.415 | 1.00 17.69 |
| ATOM | 14908 | 0 | MET | 2225 | 35.232 | -8.003 | 45.519 | 1.00 16.95 |
| ATOM | 14909 | N | LEU | 2226 | 34.411 | -10.063 | 45.866 | 1.00 17.48 |
| MOTA | 14910 | CA | LEU | 2226 | 33.228 | -9.557 | 46.547 | 1.00 17.32 |
| ATOM | 14911 | CB | LEU | 2226 | 32.245 | -10.689 | 46.819 | 1.00 16.18 |
| ATOM | 14912 | CG | LEU | 2226 | 31.283 | -11.057 | 45.681 | 1.00 14.70 |
| MOTA | 14913 | CD1 | LEU | 2226 | 30.554 | -12.330 | 46.056 | 1.00 10.61 |
| ATOM | 14914 | | LEU | 2226 | 30.287 | -9.923 | 45.438 | 1.00 15.10 |
| ATOM | 14915 | С | LEU | 2226 | 33.622 | -8.897 | 47.864 | 1.00 17.88 |
| ATOM | 14916 | 0 | LEU | 2226 | 33.203 | -7.777 | 48.158 | 1.00 16.44 |
| MOTA | 14917 | N | THR. | 2227 | 34.429 | -9.601 | 48.650 | 1.00 20.52 |
| MOTA | 14918 | CA | THR | 2227 | 34.889 | -9.099 | 49.946 | 1.00 24.25 |
| ATOM | 14919 | CB | THR | 2227 | 35.886 | -10.078 | 50.593 | 1.00 25.62 |
| ATOM | 14920 | | THR | 2227 | | -11.334 | 50.830 | 1.00 29.56 |
| MOTA | 14921 | CG2 | THR | 2227 | 36.391 | -9.524 | 51.925 | 1.00 31:43 |
| ATOM | 14922 | C | THR | 2227 | 35.543 | 7.721 | 49.851 | 1.00 24.33 |
| ATOM | 14923 | 0 | THR | 2227 | 35.235 | -6.825 | 50.643 | 1.00 25.20 |
| ATOM | 14924 | N | GLU | 2228 | 36.447 | -7.546 | 48.892 | 1.00 25.76 |
| ATOM | 14925 | CA | GLU | 2228 | 37.114 | -6.259 | 48.737 | 1.00 26.35 |
| MOTA | 14926 | CB | GLU | 2228 | 38.353 | -6.391 | 47.838 | 1.00 30.63 |
| ATOM | 14927 | CG | GLU | 2228 | 38.203 | -7.358 | 46.687 | 1.00 31.85 |
| ATOM | 14928 | CD | GLU | 2228 | 39.465 | -7.474 | 45.846 | 1.00 33.25 |
| MOTA | 14929 | | GLU | 2228 | 40.557 | -7.670 | 46.422 | 1.00 35.06 |
| MOTA | 14930 | OE2 | GLU | 2228 | 39.368 | -7.385 | 44.607 | 1.00 28.52 |
| MOTA | 14931 | C | GLU | 2228 | 36.160 | -5.202 | 48.190 | 1.00 26.51 |
| MOTA | 14932 | 0 | GLU | 2228 | 36.475 | -4.013 | 48.176 | 1.00 26.37 |
| ATOM | 14933 | N . | ARG | 2229 | 34.983 | -5.632 | 47.747 | 1.00 23.68 |
| ATOM | 14934 | CÁ | ARG | 2229 | 34.004 | -4.690 | 47.228 | 1.00 22.45 |
| MOTA | 14935 | CB | ARG | 2229 | 33.456 | -5.199 | 45.893 | 1.00 21.74 |
| ATOM | 14936 | CG | ARG | 2229 | 34.481 | -5.021 | 44.779 | 1.00 21.55 |
| ATOM | 14937 | CD | ARG | 2229 | 34.202 | -5.839 | 43.529 | 1.00 19.25 |
| MOTA | 14938 | NE | ARG | 2229 | 35.257 | -5.628 | 42.538 | 1.00 16.72 |
| MOTA | 14939 | CZ | ARG | 2229 | 36.528 | -5.998 | 42.696 | 1.00 14.29 |
| MOTA | 14940 | NH1 | ARG | 2229 | 36.918 | -6.607 | 43.804 | 1.00 14.68 |
| MOTA | 14941 | NH2 | ARG | 2229 | 37.421 | -5.745 | 41.748 | 1.00 16.15 |
| MOTA | 14942 | С | ARG | 2229. | 32.894 | -4.421 | 48.244 | 1.00 20.95 |
| MOTA | 14943 | 0 | ARG | 2229 | 31.753 | -4.099 | 47.889 | 1.00 21.04 |
| MOTA | 14944 | N | ALA | 2230 | 33.254 | -4.570 | 49.517 | 1.00 19.92 |
| MOTA | 14945 | CA | ALA | 2230 | 32.362 | -4.309 | 50.646 | 1.00 17.61 |
| MOTA | 14946 | CB | ALA | 2230 | 31.750 | -2.915 | 50.500 | 1.00 20.44 |
| MOTA | 14947 | C | ALA | 2230 | 31.265 | -5.336 | 50.912 | 1.00 18.57 |
| MOTA | 14948 | 0 | ALA | 2230 | 30.374 | -5.085 | 51.722 | 1.00 17.70 |
| MOTA | 14949 | N | VAL | 2231 | 31.335 | -6.493 | 50.254 | 1.00 17.15 |
| MOTA | 14950 | CA | VAL | 2231 | 30.324 | -7.534 | 50.444 | 1.00 17.76 |
| MOTA | 14951 | CB | VAL | 2231 | 29.729 | -8.000 | 49.083 | 1.00 17.93 |
| MOTA | 14952 | CG1 | VAL | 2231 | 28.669 | -9.075 | 49.316 | 1.00 17.35 |
| MOTA | 14953 | CG2 | VAL | 2231 | 29.125 | -6.822 | 48.335 | 1.00 17.32 |
| MOTA | 14954 | С | VAL | 2231 | 30.824 | -8.783 | 51.183 | 1.00 17.83 |
| MOTA | 14955 | 0 | VAL | 2231 | 31.576 | -9.582 | 50.623 | 1.00 18.81 |
| ATOM | 14956 | N | PRO | 2232 | 30.412 | -8.969 | 52.450 | 1.00 16.77 |
| ATOM | 14957 | CD | PRO | 2232 | 29.701 | -8.061 | 53.370 | 1.00 17.78 |
| MOTA | 14958 | CA | PRO | 2232 | 30.884 | -10.168 | 53.145 | 1.00 16.29 |
| MOTA | 14959 | CB | PRO | 2232 | 30.523 | -9.898 | 54.608 | 1.00 18.07 |
| MOTA | 14960 | CG | PRO | 2232 | 29.390 | -8.958 | 54.529 | 1.00 18.75 |
| MOTA | 14961 | С | PRO | 2232 | 30.191 | -11.391 | 52.557 | 1.00 15.35 |
| MOTA | 14962 | 0 | PRO | 2232 | 29.048 | -11.309 | 52.093 | 1.00 15.40 |
| MOTA | 14963 | N | VAL | 2233 | 30.887 | -12.520 | 52.576 | 1.00 16.70 |
| ATOM | 14964 | CA | VAL | 2233 | | -13.753 | 51.995 | 1.00 15.99 |
| MOTA | 14965 | CB | VAL | 2233 | 31.225 | -14.174 | 50.772 | 1.00 17.33 |
| MOTA | 14966 | CG1 | VAL | 2233 | 30.743 | -15.516 | 50.231 | 1.00 15.74 |

| ATOM | 14967 | CG2 | VAL | 2233 | 31.189 | -13.105 | 49.708 | 1.00 16.38 |
|--------|-------|-----------|-------|------|--------|---------|--------|------------|
| MOTA | 14968 | С | VAL | 2233 | 30.316 | -14.958 | 52.924 | 1.00 16.80 |
| ATOM | 14969 | Ö | VAL | 2233 | | -15.224 | 53.681 | 1.00 16.97 |
| | | | | | | | | |
| MOTA | 14970 | N | CYS | 2234 | | -15.695 | 52.838 | 1.00 15.58 |
| MOTA | 14971 | CA | CYS | 2234 | | -16.917 | 53.599 | 1.00 16.50 |
| MOTA | 14972 | CB | CYS | 2234 | 27.683 | -16.974 | 54.281 | 1.00 15.73 |
| ATOM | 14973 | SG | CYS | 2234 | 27.369 | -18.518 | 55.159 | 1.00 16.61 |
| ATOM | 14974 | С | CYS | 2234 | 29.140 | -18.027 | 52.552 | 1.00 18.28 |
| ATOM | 14975 | ō | CYS | 2234 | - | -17.992 | 51.544 | 1.00 19.80 |
| | 14976 | N | GLY | 2235 | | -18.990 | 52.775 | 1.00 17.80 |
| ATOM | | | | | | | | |
| MOTA | 14977 | CA | GLY | 2235 | | -20.093 | 51.841 | 1.00 17.79 |
| MOTA | 14978 | С | GLY | 2235 | | -21.125 | 52.090 | 1.00 16.39 |
| MOTA | 14979 | 0 | GLY | 2235 | | -21.021 | 53.060 | 1.00 16.55 |
| ATOM | 14980 | N | HIS | 2236 | 28.989 | -22.123 | 51.219 | 1.00 16.49 |
| ATOM | 14981 | CA | HIS | 2236 | 27.981 | -23.169 | 51.378 | 1.00 19.27 |
| ATOM | 14982 | CB | HIS | 2236 | | -22.690 | 50.790 | 1.00 19.17 |
| MOTA | 14983 | CG | HIS | 2236 | | -23.600 | 51.058 | 1.00 20.45 |
| | | | HIS | 2236 | | -24.925 | 51.334 | 1.00 21.15 |
| MOTA | 14984 | | | | | | | |
| MOTA | 14985 | | HIS | 2236 | | -23.163 | 51.018 | 1.00 20.57 |
| MOTA | 14986 | | HIS | 2236 | | -24.178 | 51.258 | 1.00 20.23 |
| MOTA | 14987 | NE2 | HIS | 2236 | 24.107 | -25.260 | 51.454 | 1.00 19.86 |
| ATOM | 14988 | С | HIS | 2236 | 28.480 | -24.420 | 50.667 | 1.00 19.78 |
| ATOM | 14989 | 0 | HIS | 2236 | 28.538 | -24.463 | 49.438 | 1.00 18.95 |
| ATOM | 14990 | N | LEU | 2237 | 28 849 | -25.427 | 51.455 | 1.00 21.72 |
| MOTA | 14991 | CA | LEU | 2237 | | -26.686 | 50.926 | 1.00 22.90 |
| | | | | | | | | |
| ATOM | 14992 | CB | LEU | 2237 | 30.823 | -26.880 | 51.383 | 1.00 21.03 |
| ATOM | 14993 | CG | LEU | 2237 | | -25.837 | 50.920 | 1.00 21.00 |
| MOTA . | 14994 | | LEU | 2237 | | -26.144 | 51.536 | 1.00 20.20 |
| MOTA | 14995 | CD2 | LEU | 2237 | 31.942 | -25.844 | 49.401 | 1.00 22.91 |
| ATOM | 14996 | С | LEU | 2237 | 28.542 | -27.881 | 51.365 | 1.00 22.62 |
| ATOM | 14997 | 0 | LEU | 2237 | 27,701 | -27.768 | 52.256 | 1.00 22.68 |
| MOTA | 14998 | N | GLY | 2238 | | -29.028 | 50.739 | 1.00 23.03 |
| ATOM | 14999 | CA | GLY | 2238 | | -30.235 | 51.061 | 1.00 22.71 |
| | | | | | | | | |
| MOTA | 15000 | C | GLY | 2238 | | -30.398 | 50.096 | 1.00 24.92 |
| ATOM | 15001 | 0 | GLY | 2238 | | -30.367 | 48.880 | 1.00 24.62 |
| MOTA | 15002 | . N | LEU | 2239 | | -30.565 | 50.631 | 1.00 25.75 |
| MOTA | 15003 | CA | LEU | 2239 | 24.506 | -30.715 | 49.801 | 1.00 27.14 |
| ATOM | 15004 | CB | LEU | 2239 | 23.427 | -31.485 | 50.573 | 1.00 27.64 |
| ATOM | 15005 | CG | LEU | 2239 | | -32.031 | 49.822 | 1.00 29.36 |
| MOTA | 15006 | | LEU | 2239 | | -32.870 | 50.782 | 1.00 29.18 |
| ATOM | 15007 | | LEU | 2239 | | -30.905 | 49.248 | 1.00 29.54 |
| | | | | | | | | |
| MOTA | 15008 | С | LEU | 2239 | | -29.323 | 49.416 | 1.00 27.73 |
| MOTA | 15009 | 0 | LEU . | | | -28.681 | 50.181 | 1.00 29.81 |
| MOTA | 15010 | N | THR | 2240 | | -28.866 | 48.231 | 1.00 24.58 |
| MOTA | 15011 | CA | THR | 2240 | 23.998 | -27.559 | 47.714 | 1.00 24.57 |
| ATOM | 15012 | CB | THR | 2240 | 25.156 | -26.932 | 46.894 | 1.00 25.13 |
| ATOM | 15013 | OG1 | | 2240 | 25.600 | -27.858 | 45.890 | 1.00 23.49 |
| ATOM | 15014 | CG2 | THR | 2240 | | -26.607 | 47.810 | 1.00 26.36 |
| | | C | THR | 2240 | | -27.721 | 46.840 | 1.00 24.62 |
| ATOM | 15015 | | | | | | | - |
| ATOM | 15016 | 0 | THR | 2240 | | -28.055 | 45.661 | 1.00 23.83 |
| MOTA | | N | PRO | 2241 | | -27.473 | 47.420 | 1.00 24.68 |
| MOTA | 15018 | CD | PRO | 2241 | | -26.858 | 48.749 | 1.00 25.30 |
| ATOM | 15019 | CA | PRO | 2241 | 20.267 | -27.592 | 46.741 | 1.00 24.86 |
| ATOM | 15020 | CB ` | PRO | 2241 | 19.283 | -27.004 | 47.758 | 1.00 24.84 |
| ATOM | 15021 | CG | PRO | 2241 | 20.136 | -26.080 | 48.575 | 1.00 27.84 |
| ATOM | 15022 | С | PRO | 2241 | | -27.002 | 45.337 | 1.00 24.57 |
| ATOM | 15022 | Õ | PRO | 2241 | | -27.530 | 44.534 | 1.00 24.58 |
| | | | | | | -25.924 | 45.026 | |
| MOTA | 15024 | N | GLN | 2242 | | | | 1.00 22.22 |
| MOTA | 15025 | CA | GLN | 2242 | | -25.335 | 43.687 | 1.00 22.19 |
| MOTA | 15026 | СВ | GLN | 2242 | | -24.064 | | 1.00 21.42 |
| ATOM | 15027 | CG | GLN | 2242 | 20.849 | -22.785 | 43.987 | 1.00 19.29 |
| ATOM | 15028 | CD | GLN | 2242 | 21.784 | -21.601 | 44.191 | 1.00 20.80 |
| ATOM | 15029 | | GLN | 2242 | 22.795 | -21.460 | 43.498 | 1.00 18.83 |
| ATOM | 15030 | | GLN | 2242 | | -20.736 | 45.140 | 1.00 17.73 |
| ATOM | 15031 | C | GLN | 2242 | | -26.331 | 42.602 | 1.00 21.96 |
| ATOM | 15031 | Õ | GLN | 2242 | | -26.261 | 41.470 | 1.00 20.71 |
| | | | | 2242 | | -27.259 | 42.962 | |
| ATOM | 15033 | N . | SER | | | | | 1.00 20.88 |
| ATOM | 15034 | CA | SER | 2243 | | -28.271 | 42.032 | 1.00 20.30 |
| MOTA | 15035 | CB | SER | 2243 | | -28.559 | 42.293 | 1.00 20.51 |
| MOTA | 15036 | OG | SER | 2243 | | -27.405 | 42.099 | 1.00 18.03 |
| MOTA | 15037 | С | SER | 2243 | 21.772 | -29.587 | 42.140 | 1.00 20.10 |
| MOTA | 15038 | 0 | SER | 2243 | 22.281 | -30.647 | 41.764 | 1.00 19.42 |
| ATOM | 15039 | N | VAL | 2244 | | -29.519 | 42.633 | 1.00 20.27 |
| ATOM | 15040 | CA | VAL | 2244 | | -30.712 | 42.806 | 1.00 19.69 |
| ATOM | | | | 2244 | | -30.340 | 43.313 | 1.00 20.85 |
| | 15041 | CB CC1 | VAL | | | | | |
| ATOM | 15042 | | VAL | 2244 | | -29.559 | 42.245 | 1.00 19.91 |
| MOTA | 15043 | CG2 | VAL | 2244 | 11.525 | -31.601 | 43.698 | 1.00 21.83 |
| | | | | | | | | |

| ATOM | 15044 | С | VAL | 2244 | 19.581 | -31.558 | 41.538 | 1.00 | 20.01 |
|--------------|----------------|------------|------------|--------------|--------|--------------------|------------------|------|----------------|
| ATOM | 15045 | 0 | VAL | 2244 | 19.484 | -32.785 | 41.611 | 1.00 | 19.12 |
| ATOM | 15046 | N | ASN | 2245 | | -30.907 | 40.379 | 1.00 | 17.97 |
| MOTA | 15047 | CA | ASN | 2245 | | -31.626 | 39.118 | 1.00 | 19.30 |
| MOTA | 15048 | CB | ASN | 2245 | | -30.653 | 37.993 | 1.00 | 17.46 |
| ATOM | 15049 | CG OD1 | ASN ASN | 2245 2245 | | -30.102 -30.850 | 38.146 38.058 | 1.00 | 19.80 16.40 |
| MOTA MOTA | 15050 15051 | | ASN | 2245 | 17.601 | -28.796 | 38.386 | | 18.40 |
| ATOM | 15052 | C | ASN | 2245 | | -32.367 | 38.787 | 1.00 | 19.89 |
| ATOM | 15053 | 0 | ASN | 2245 | | -33.401 | 38.114 | 1.00 | 20.19 |
| MOTA | 15054 | N | ILE | 2246 | 21.881 | -31.835 | 39.254 | 1.00 | 20.52 |
| MOTA | 15055 | CA | ILE | 2246 | | -32.482 | 39.011 | 1.00 | |
| ATOM | 15056 | CB | ILE | 2246 | | -31.581 | 39.411 | | 20.68 |
| ATOM | 15057 | CG2 | ILE ILE | 2246 | | -32.401 -30.365 | 39.365 38.472 | | 21.13 20.19 |
| ATOM ATOM | 15058 15059 | CG1 | ILE | 2246 2246 | | -30.365 | 37.085 | 1.00 | 18.99 |
| ATOM | 15060 | C | ILE | 2246 | | -33.759 | 39.847 | 1.00 | 22.01 |
| ATOM | 15061 | 0 | ILE | 2246 | | -34.821 | 39.333 | 1.00 | 21.51 |
| ATOM | 15062 | N | PHE | 2247 | 22.953 | -33.647 | 41.136 | | 22.01 |
| ATOM | 15063 | CA | PHE | 2247 | | -34.796 | 42.036 | | 24.57 |
| MOTA | 15064 | CB | PHE | 2247 | | -34.351 | 43.498 | 1.00 | 27.03 |
| MOTA | 15065 | CG CD1 | PHE. | 2247 | | -33.243 | 43.852 43.522 | 1.00 | 30.51 |
| MOTA MOTA | 15066 15067 | | PHE PHE | 2247 2247 | | -33.328 -32.113 | 44.530 | | 32.37 |
| ATOM | 15068 | | PHE | 2247 | | -32.302 | 43.860 | | 33.67 |
| ATOM | 15069 | | PHE | 2247 | | -31.082 | 44.873 | | 34.16 |
| MOTA | 15070 | CZ | PHE | 2247 | 25.667 | -31.174 | 44.538 | 1.00 | 34.12 |
| ATOM | 15071 | С | PHE | 2247 | | -35.806 | 41.779 | | 24.16 |
| - | 15072 | 0 | PHE | 2247 | 22.042 | -36.975 | 42.136 | 1.00 | 25.60 |
| ATOM | 15073 | N | GLY | 2248 | | -35.349 | 41.166 | 1.00 | 22.84 |
| MOTA MOTA | 15074 15075 | CA C | GLY GLY | 2248 2248 | | -36.233 -36.384 | 40.893 42.107 | 1.00 | 23.98 25.53 |
| MOTA | 15076 | 0 | GLY | 2248 | | -37.362 | 42.238 | 1.00 | 25.77 |
| ATOM | 15077 | N | GLY | 2249 | | -35.405 | 43.002 | 1.00 | |
| MOTA | 15078 | CA | GLY | 2249 | | -35.442 | 44.209 | 1.00 | 29.60 |
| MOTA | 15079 | C | GLY | 2249 | | -34.872 | 45.387 | | 31.46 |
| MOTA | 15080 | 0 | GLY | 2249 2250 | 19.994 | -34.452 -34.848 | 45.241 46.553 | | 31.11 |
| MOTA MOTA | 15081 15082 | N CA | TYR TYR | 2250 | 18.843 | -34.330 | 47.758 | 1.00 | |
| ATOM | 15083 | CB | TYR | 2250 | | -33.608 | 48.638 | | 38.09 |
| ATOM | 15084 | CG | TYR | 2250 | 17.136 | -32.453 | 47.945 | 1.00 | 40.93 |
| MOTA | 15085 | CD1 | | 2250 | | -32.640 | 47.243 | | 41.37 |
| ATOM | 15086 | CE1 | | 2250 | | -31.580 -31.174 | 46.584 47.970 | | 43.82 |
| MOTA MOTA | 15087 15088 | CD2 CE2 | TYR TYR | 2250 2250 | | -30.108 | 47.314 | | 43.92 |
| ATOM | 15089 | CZ | TYR | 2250 | 15.902 | -30.317 | 46.624 | | 43.98 |
| ATOM | 15090 | OH | TYR | 2250 | 15.303 | -29.264 | 45.971 | 1.00 | 45.48 |
| MOTA | 15091 | C | TYR | 2250 | | -35.477 | 48.528 | | 37.32 |
| ATOM | 15092 | 0 | TYR | 2250 2251 | | -36.090 -35.755 | 49.392 48.204 | 1.00 | 38.37 37.64 |
| MOTA MOTA | 15093 15094 | N CA | LYS LYS | 2251 | | -36.839 | 48.830 | 1.00 | |
| ATOM | 15095 | CB | LYS | 2251 | | -37.776 | 47.742 | | 37.65 |
| MOTA | 15096 | CG | LYS | 2251 | 20.954 | -38.168 | 46.711 | 1.00 | 37.38 |
| MOTA | 15097 | CD | LYS | 2251 | | -38.742 | 45.448 | | 37.94 |
| ATOM | 15098 | CE | LYS | 2251 | | -39.094 -39.517 | 44.415 43.119 | | 37.48 33.97 |
| MOTA MOTA | 15099 15100 | NZ C | LYS LYS | 2251 2251 | | -36.287 | 49.659 | | 37.97 |
| MOTA | 15101 | 0 | LYS | 2251 | | -35.221 | 49.358 | | 36.96 |
| ATOM | 15102 | N | VAL | 2252 | 23.012 | -37.018 | 50.706 | 1.00 | 37.82 |
| MOTA | 15103 | CA | VAL | 2252 | | -36.605 | 51.576 | | 39.23 |
| ATOM | 15104 | CB | VAL | 2252 | | -37.621 -37.137 | 52.717 53.651 | | 38.53 |
| MOTA MOTA | 15105 15106 | CG1 | VAL VAL | 2252 2252 | | -37.137 | 53.479 | | 39.33 |
| ATOM | 15107 | C | VAL | 2252 | | -36.497 | 50.759 | | 39.59 |
| ATOM | 15108 | Ō | VAL | 2252 | | -37.240 | 49.798 | | 39.94 |
| MOTA | 15109 | N | GLN | 2253 | | -35.574 | 51.144 | | 40.19 |
| MOTA | 15110 | CA | GLN | 2253 | | -35.376 | 50.430 | | 41.92 |
| ATOM MOTA | 15111 15112 | CB CG | GLN GLN | 2253 2253 | | -34.008 -33.976 | 49.743 48.384 | | 42.02 43.44 |
| ATOM | 15112 | CD | GLN | 2253 | | -34.825 | 47.349 | | 42.91 |
| ATOM | 15114 | | GLN | 2253 | | -34.672 | 47.128 | | 43.91 |
| MOTA | 15115 | NE2 | | 2253 | | -35.723 | 46.704 | | 44.45 |
| ATOM | 15116 | С | GLN | 2253 | | -35.469 | 51.398 | | 42.35 |
| ATOM ATOM | 15117 15118 | O N | GLN GLY | 2253 2254 | | -35.358 -35.677 | 52.610 50.862 | | 42.17 43.70 |
| ATOM | 15110 | CA | GLY | 2254 | | -35.779 | 51.709 | | 45.07 |
| ATOM | 15120 | С | GLY | 2254 | | -37.209 | 52.071 | | 46.95 |

| ATOM | 15121 | 0 | GLY | 2254 | 32.521 -37.466 | 52.581 | 1.00 47.08 |
|-------|--------------------|-----|----------------------|------|----------------|--------|------------|
| ATOM | 15122 | N | ARG | 2255 | 30.517 -38.140 | 51.814 | 1.00 48.47 |
| ATOM | 15123 | CA | ARG | 2255 | 30.742 -39.552 | 52.105 | 1.00 49.93 |
| ATOM | 15124 | CB | ARG | 2255 | 29.517 -40.378 | 51.696 | 1.00 50.98 |
| | | | | | 28.224 -40.026 | | |
| ATOM | 15125 | CG | ARG | 2255 | | 52.424 | |
| ATOM | 15126 | CD | ARG | 2255 | 28.282 -40.425 | 53.887 | 1.00 52.47 |
| ATOM | 15127 | NE | ARG | 2255 | 27.032 -40.148 | 54.596 | 1.00 53.65 |
| MOTA | 15128 ⁻ | CZ | ARG | 2255 | 25.864 -40.724 | 54.322 | 1.00 52.93 |
| ATOM | 15129 | NH1 | ARG | 2255 | 25.768 -41.618 | 53.349 | 1.00 52.83 |
| ATOM | 15130 | NH2 | ARG | 2255 | 24.786 -40.409 | 55.027 | 1.00 53.44 |
| ATOM | 15131 | С | ARG | 2255 | 31.966 -40.058 | 51.342 | 1.00 50.92 |
| ATOM | 15132 | ō | ARG | 2255 | 31.965 -40.097 | 50.111 | 1.00 50.96 |
| ATOM | 15133 | N | GLY | 2256 | 33.010 -40.444 | 52.070 | 1.00 51.41 |
| | | | | | | | 1.00 51.41 |
| MOTA | 15134 | CA | GLY | 2256 | 34.211 -40.938 | 51.419 | |
| MOTA | 15135 | С | GLY | 2256 | 35.428 -40.069 | 51.677 | 1.00 52.97 |
| MOTA | 15136 | 0 | GLY | 2256 | 35.313 -38.854 | 51.819 | 1.00 52.71 |
| MOTA | 15137 | N | ASP | 2257 | 36.599 -40.694 | 51.732 | 1.00 53.48 |
| ATOM | 15138 | CA | ASP | 2257 | 37.838 -39.969 | 51.982 | 1.00 53.79 |
| ATOM | 15139 | CB | ASP | 2257 | 39.023 -40.934 | 52.009 | 1.00 55.06 |
| ATOM | 15140 | CG | ASP | 2257 | 38.901 -41.970 | 53.105 | 1.00 56.30 |
| ATOM | 15141 | | ASP | 2257 | 38.722 -41.576 | 54.277 | 1.00 56.85 |
| ATOM | 15142 | OD2 | | 2257 | 38.987 -43.177 | 52.797 | 1.00 58.02 |
| ATOM | 15143 | C | ASP | 2257 | 38.084 -38.893 | 50.935 | 1.00 53.11 |
| | | | | | | 51.269 | |
| ATOM | 15144 | 0 | ASP | 2257 | 38.356 -37.741 | | 1.00 53.00 |
| MOTA | 15145 | N | GLU | 2258 | 37.989 -39.273 | 49.666 | 1.00 52.48 |
| MOTA | 15146 | CA | GLU | 2258 | 38.213 -38.335 | 48.576 | 1.00 51.39 |
| MOTA | 15147 | CB | GLU | 2258 | 38.123 -39.062 | 47.234 | 1.00 53.26 |
| MOTA | 15148 | CG | GLU | 2258 | 38.351 -38.169 | 46.028 | 1.00 55.82 |
| MOTA | 15149 | CD | GLU | 2258 | 38.623 -38.959 | 44.762 | 1.00 57.62 |
| ATOM | 15150 | OE1 | GLU | 2258 | 39.678 -39.629 | 44.695 | 1.00 58.68 |
| ATOM | 15151 | OE2 | | 2258 | 37.783 -38.913 | 43.837 | 1.00 58.41 |
| ATOM | 15152 | C | GLU | 2258 | 37.210 -37.188 | 48.620 | 1.00 49.36 |
| ATOM | 15152 | o | GLU | 2258 | 37.591 -36.020 | 48.567 | 1.00 48.74 |
| | | | | | | | |
| MOTA | 15154 | N | ALA | 2259 | 35.929 -37.527 | 48.721 | 1.00 47.48 |
| MOTA | 15155 | CA | ALA | 2259 | 34.877 -36.521 | 48.778 | 1.00 45.65 |
| MOTA | 15156 | CB | ALA | 2259 | 33.510 -37.191 | 48.747 | 1.00 45.32 |
| MOTA | 15157 | C | ALA | 2259 | 35.023 -35.688 | 50.046 | 1.00 43.78 |
| MOTA | 15158 | O | ALA | 2259 | 34.742 -34.491 | 50.047 | 1.00 43.87 |
| ATOM | 15159 | N | GLY | 2260 | 35.466 ~36.330 | 51.121 | 1.00 42.56 |
| MOTA | 15160 | CA | GLY | 2260 | 35.644 ÷35.632 | 52.380 | 1.00 41.13 |
| ATOM | 15161 | С | GLY | 2260 | 36.794 -34.645 | 52.338 | 1.00 40.59 |
| ATOM | 15162 | ō | GLY | 2260 | 36.680 -33.524 | 52.837 | 1.00 39.79 |
| ATOM | 15163 | N | ASP | 2261 | 37.909 -35.056 | 51.744 | 1.00 38.76 |
| | | | | | | | 1.00 38.76 |
| ATOM | 15164 | CA | ASP | 2261 | 39.070 -34.182 | 51.647 | |
| MOTA | 15165 | CB | ASP | 2261 | 40.291 -34.959 | 51.141 | 1.00 39.33 |
| MOTA | 15166 | CG | ASP | 2261 | 40.635 -36.142 | 52.025 | 1.00 40.38 |
| MOTA | 15167 | | ASP | 2261 | 40.613 -35.990 | 53.267 | 1.00 39.92 |
| ATOM | 15168 | OD2 | ASP | 2261 | 40.938 -37.224 | 51.477 | 1.00 42.70 |
| MOTA | 15169 | С | ASP | 2261 | 38.775 -33.022 | 50.707 | 1.00 36.18 |
| MOTA | 15170 | 0 | ASP | 2261 | 39.279 -31.915 | 50.899 | 1.00 35.73 |
| MOTA | 15171 | N | GLN | 2262 | 37.951 -33.279 | 49.695 | 1.00 35.55 |
| ATOM | 15172 | CA | GLN | 2262 | 37.588 -32.246 | 48.728 | 1.00 34.77 |
| ATOM | 15173 | СВ | GLN | 2262 | 36.718 -32.844 | 47.617 | 1.00 35.12 |
| ATOM | 15174 | CG | GLN | 2262 | 36.351 -31.864 | 46.504 | 1.00 37.06 |
| ATOM | 15175 | CD | GLN | 2262 | 37.568 -31.284 | 45.803 | 1.00 38.05 |
| ATOM | 15175 | OE1 | | 2262 | 38.409 -32.019 | 45.281 | 1.00 39.24 |
| | | | | | | | |
| ATOM | 15177 | NE2 | | 2262 | 37.665 -29.960 | 45.782 | 1.00 38.19 |
| ATOM | 15178 | C | GLN | 2262 | 36.839 -31.112 | 49.422 | 1.00 33.47 |
| ATOM | 15179 | 0 | GLN | 2262 | 37.118 -29.939 | 49.177 | 1.00 33.28 |
| MOTA | 15180 | N | LEU | 2263 | 35.888 -31.469 | 50.284 | 1.00 32.83 |
| ATOM | 15181 | CA | LEU | 2263 | 35.105 -30.478 | 51.020 | 1.00 31.73 |
| MOTA | 15182 | CB | LEU | 2263 | 33.968 -31.153 | 51.796 | 1.00 32.63 |
| ATOM | 15183 | CG | LEU | 2263 | 32.813 -31.739 | 50.973 | 1.00 35.13 |
| ATOM | 15184 | | LEU | 2263 | 31.733 -32.282 | 51.905 | 1.00 36.24 |
| ATOM | 15185 | | LEU | 2263 | 32.230 -30.652 | 50.073 | 1.00 35.79 |
| ATOM | 15186 | C | LEU | 2263 | 35.993 -29.701 | 51.986 | 1.00 30.80 |
| ATOM. | 15187 | 0 . | LEU | 2263 | 35.874 -28.484 | 52.110 | 1.00 30.26 |
| MOTA | 15188 | N | LEU | 2264 | 36.883 -30.408 | 52.674 | 1.00 30.20 |
| | | | | | | | |
| ATOM | 15189 | CA | LEU | 2264 | 37.789 -29.762 | 53.613 | 1.00 28.33 |
| ATOM | 15190 | CB | LEU | 2264 | 38.704 -30.804 | 54.259 | 1.00 31.47 |
| MOTA | 15191 | ÇG | LEU | 2264 | 39.283 -30.483 | 55.639 | 1.00 33.11 |
| MOTA | 15192 | | LEU | 2264 | 40.170 -31.648 | 56.068 | 1.00 32.67 |
| MOTA | 15193 | | LEU | 2264 | 40.069 -29.188 | 55.623 | 1.00 33.38 |
| MOTA | 15194 | С | LEU | 2264 | 38.631 -28.742 | 52.855 | 1.00 26.63 |
| MOTA | 15195 | 0 | LEU | 2264 | 38.761 -27.594 | 53.275 | 1.00 26.53 |
| MOTA | 15196 | N | SER | 2265 | 39.198 -29.170 | 51.732 | 1.00 25.34 |
| MOTA | 15197 | CA | SER | 2265 | 40.029 -28.291 | 50.918 | 1.00 25.06 |
| | | - | | | | | 3.00 |

| ATOM | 15198 | СВ | SER | 2265 | 40.546 | -29.036 | 49.686 | 1.00 25.94 |
|--------------|-------|--------|-----|--------------|--------|---------|--------|--------------------------|
| ATOM | 15199 | OG | SER | 2265 | | -28.193 | 48.895 | 1.00 26.74 |
| ATOM | 15200 | c | SER | 2265 | | -27.067 | 50.475 | 1.00 24.21 |
| ATOM | 15201 | 0 | SER | 2265 | | -25.945 | 50.524 | 1.00 22.95 |
| ATOM | 15202 | N | ASP | 2266 | | -27.296 | 50.044 | 1.00 23.92 |
| ATOM | 15203 | CA | ASP | 2266 | | -26.215 | 49.594 | 1.00 24.88 |
| ATOM | 15204 | CB | ASP | 2266 | | -26.776 | 49.045 | 1.00 25.99 |
| ATOM | 15205 | CG | ASP | 2266 | - | -27.401 | 47.671 | 1.00 29.42 |
| ATOM | 15206 | | ASP | 2266 | | -26.744 | 46.775 | 1.00 31.95 |
| | 15207 | | ASP | 2266 | | -28.545 | 47.478 | 1.00 34.49 |
| MOTA | 15207 | C | ASP | 2266 | | -25.231 | 50.724 | 1.00 22.16 |
| ATOM ATOM | 15209 | 0 | ASP | 2266 | | -24.013 | 50.529 | 1.00 22.29 |
| | 15210 | N | ALA | 2267 | | -25.767 | 51.902 | 1.00 22.20 |
| MOTA | 15211 | ĊA | ALA | 2267 | | -24.944 | 53.069 | 1.00 20.33 |
| ATOM | | CB | ALA | 2267 | | -25.836 | 54.280 | 1.00 19.05 |
| ATOM | 15212 | | | | | -24.021 | 53.354 | 1.00 10.03 |
| MOTA | 15213 | C | ALA | 2267 | | -22.817 | 53.546 | 1.00 20.70 |
| MOTA | 15214 | 0 | ALA | 2267 | | -24.584 | 53.348 | 1.00 19.57 |
| MOTA | 15215 | N | LEU | 2268 | | | 53.629 | 1.00 19.37 |
| ATOM | 15216 | CA | LEU | 2268 | | -23.781 | | |
| ATOM | 15217 | CB | LEU | 2268 | | -24.671 | 53.712 | 1.00 22.33 |
| MOTA | 15218 | CG | LEU | 2268 | | -25.470 | 54.997 | 1.00 23.44 |
| MOTA | 15219 | | LEU | 2268 | | -26.428 | 54.850 | 1.00 24.11 |
| MOTA | 15220 | | LEU | 2268 | | -24.519 | 56.173 | 1.00 23.26 |
| MOTA | 15221 | C | LEU | 2268 | | -22.736 | 52.544 | 1.00 21.76 |
| MOTA | 15222 | 0 | LEU | 2268 | | -21.600 | 52.837 | 1.00 23.46 |
| MOTA | 15223 | N | ALA | 2269 | | -23.120 | 51.295 | 1.00 21.45 |
| MOTA | 15224 | CA | ALA | 2269 | | -22.204 | 50.174 | 1.00 22.17 |
| ATOM | 15225 | CB | ALA | 2269 | | -22.938 | 48.853 | 1.00 22.22 |
| MOTA | 15226 | C | ALA | 2269 | 39.000 | -21.015 | 50.283 | 1.00 21.51 |
| MOTA | 15227 | 0 | ALA | 2269 | | -19.871 | 50.061 | 1.00 21.07 |
| MOTA | 15228 | N | LEU | 2270 | 37.745 | -21.285 | 50.620 | 1.00 19.82 |
| ATOM | 15229 | CA | LEU | 2270 | 36.761 | -20.215 | 50.753 | 1.00 21.19 |
| ATOM | 15230 | CB | LEU | 2270 | 35.377 | -20.804 | 51.028 | 1.00 19.10 |
| MOTA | 15231 | CG | LEU | 2270 | 34.777 | -21.647 | 49.897 | 1.00 20.93 |
| MOTA | 15232 | CD1 | LEU | 2270 | 33.488 | -22.306 | 50.382 | 1.00 20.19 |
| MOTA | 15233 | | LEU | 2270 | 34.509 | -20.763 | 48.682 | 1.00 20.41 |
| ATOM | 15234 | С | LEU | 2270 | 37.162 | -19.269 | 51.882 | 1.00 20.84 |
| ATOM | 15235 | 0 | LEU | 2270 | | -18.050 | 51.761 | 1.00 21.29 |
| ATOM | 15236 | N | GLU | 2271 | 37.644 | -19.834 | 52.982 | 1.00 22.99 |
| ATOM | 15237 | CA | GLU | 2271 | 38.072 | -19.022 | 54.111 | 1.00 22.49 |
| ATOM | 15238 | СВ | GLU | 2271 | | -19.919 | 55.277 | 1.00 23.48 |
| ATOM | 15239 | CG | GLU | 2271 | 39.110 | -19.168 | 56.431 | 1.00 24.86 |
| ATOM | 15240 | CD | GLU | 2271 | | -20.086 | 57.555 | 1.00 27.13 |
| MOTA | 15241 | | GLU | 2271 | | -21.059 | 57.280 | 1.00 26.64 |
| MOTA | 15242 | | GLU | 2271 | | -19.831 | 58.710 | 1.00 25.55 |
| ATOM | 15243 | C | GLU | 2271 | 39.241 | | 53.704 | 1.00 22.11 |
| ATOM | 15244 | ō | GLU | 2271 | 39.270 | -16.943 | 54.018 | 1.00 22.92 |
| ATOM | 15245 | N | ALA | 2272 | | -18.703 | 52.992 | 1.00 23.39 |
| ATOM | 15246 | CA | ALA | 2272 | | -17.938 | 52.558 | 1.00 23.06 |
| ATOM | 15247 | CB | ALA | 2272 | | -18.878 | 51.946 | 1.00 23.50 |
| ATOM | 15248 | C | ALA | 2272 | | -16.855 | 51.557 | 1.00 23.55 |
| ATOM | 15249 | ō | ALA | 2272 | | -15.826 | 51.455 | 1.00 23.19 |
| ATOM | 15250 | N | ALA | 2273 | | -17.091 | 50.821 | 1.00 23.38 |
| ATOM | 15251 | CA | ALA | 2273 | | -16.135 | 49.826 | 1.00 22.05 |
| ATOM | 15252 | CB | ALA | 2273 | | -16.824 | 48.864 | 1.00 21.44 |
| | 15253 | | ALA | 2273 | | -14.935 | 50.481 | 1.00 21.79 |
| ATOM ATOM | 15254 | C O | ALA | 2273 | | -13.908 | 49.839 | 1.00 21.79 |
| | 15255 | N | GLY | 2274 | | -15.066 | 51.758 | 1.00 21.57 |
| ATOM ATOM | 15256 | CA | GLY | 2274 | | -13.961 | 52.445 | 1.00 21.55 |
| | | C | | 2274 | | -14.262 | 53.078 | 1.00 21.17 |
| MOTA | 15257 | | GLY | | | -13.392 | 53.725 | 1.00 21.65 |
| MOTA | 15258 | O | GLY | 2274 2275 | | | 52.898 | 1.00 22.32 |
| MOTA | 15259 | N | ALA | | | -15.475 | | |
| MOTA | 15260 | CA | ALA | 2275 | | -15.831 | 53.489 | 1.00 20.83 1.00 22.14 |
| ATOM | 15261 | CB | ALA | 2275 | | -17.257 | 53.107 | |
| ATOM | 15262 | C | ALA | 2275 | | -15.698 | 55.010 | 1.00 21.17 |
| MOTA | 15263 | 0 | ALA | 2275 | 35.616 | -16.184 | 55.634 | 1.00 20.62 |
| ATOM | 15264 | N | GLN | 2276 | 33.684 | -15.039 | 55.604 | 1.00 21.24 |
| ATOM | 15265 | CA | GLN | 2276 | | -14.850 | 57.051 | 1.00 21.02 |
| ATOM | 15266 | CB | GLN | 2276 | 33.293 | -13.402 | 57.378 | 1.00 22.86 |
| MOTA | 15267 | CG | GLN | 2276 | | -12.396 | 56.843 | 1.00 24.47 |
| MOTA | 15268 | CD | GLN | 2276 | | -10.954 | 57.096 | 1.00 27.97 |
| ATOM | 15269 | OE1 | | 2276 | | -10.441 | 58.212 | 1.00 29.78 |
| ATOM | 15270 | NE2 | GLN | 2276 | | -10.292 | 56.055 | 1.00 27.80 |
| ATOM | 15271 | C | GLN | 2276 | | -15.817 | 57.752 | 1.00 20.18 |
| ATOM | 15272 | 0 | GLN | 2276 | | -15.819 | 58.978 | 1.00 18.91 |
| MOTA | 15273 | N | LEU | 2277 | | -16.645 | 56.961 | 1.00 18.68 |
| ATOM | 15274 | CA | LEU | 2277 | 31.113 | -17.638 | 57.480 | 1.00 19.05 |

| ATOM | 15275 | СВ | LEU | 2277 | 29.735 | -17.009 | 57.677 | 1.00 21.48 |
|--------------|----------------|-----------|------------|--------------|--------|--------------------|------------------|--------------------------|
| ATOM | 15276 | CG | LEU | 2277 | | -16.728 | 59.113 | 1.00 23.83 |
| ATOM | 15277 | | LEU | 2277 | | -15.939 | 59.098 | 1.00 24.53 |
| ATOM | 15278 | CD2 | LEU | 2277 | | -18.040 | 59.848 | 1.00 26.07 |
| ATOM | 15279 | С | LEU | 2277 | 30.996 | -18.787 | 56.485 | 1.00 18.50 |
| ATOM | 15280 | 0 | LEU | 2277 | 31.197 | -18.591 | 55.291 | 1.00 19.06 |
| ATOM | 15281 | N | LEU | 2278 | 30.669 | -19.978 | 56.978 | 1.00 19.37 |
| ATOM | 15282 | CA | LEU | 2278 | 30.511 | -21.141 | 56.114 | 1.00 20.54 |
| ATOM | 15283 | CB | LEU | 2278 | 31.795 | -21.980 | 56.080 | 1.00 21.74 |
| ATOM | 15284 | CG | LEU | 2278 | 31.702 | -23.321 | 55.329 | 1.00 23.36 |
| ATOM | 15285 | CD1 | LEU | 2278 | 31.185 | -23.110 | 53.910 | 1.00 21.69 |
| ATOM | 15286 | CD2 | LEU | 2278 | 33.070 | -23.977 | 55.307 | 1.00 23.09 |
| MOTA | 15287 | С | LEU | 2278 | 29.367 | -22.036 | 56.560 | 1.00 20.51 |
| MOTA | 15288 | 0 | LEU | 2278 | | -22.346 | 57.746 | 1.00 19.68 |
| MOTA | 15289 | N | VAL | 2279 | | -22.451 | 55.607 | 1.00 19.72 |
| MOTA | 15290 | CA | VAL | 2279 | | -23.340 | 55.909 | 1.00 20.12 |
| MOTA | 15291 | CB | VAL | 2279 | | -22.829 | 55.295 | 1.00 19.59 |
| ATOM | 15292 | | VAL | 2279 | | -23.929 | 55.348 | 1.00 21.46 |
| MOTA | 15293 | | VAL | 2279 | | -21.615 | 56.063 | 1.00 17.21 |
| ATOM | 15294 | С | VAL | 2279 | | -24.731 | 55.354 | 1.00 19.77 |
| MOTA | 15295 | 0 | VAL | 2279 | | -24.878 | 54.202 | 1.00 20.28 |
| MOTA | 15296 | N | LEU | 2280 | | -25.744 | 56.191 | 1.00 18.40 |
| ATOM | 15297 | CA | LEU | 2280 | | -27.133 | 55.787 | 1.00 19.76 |
| ATOM | 15298 | CB | LEU LEU | 2280 | | -27.847 -27.418 | 56.717 56.656 | 1.00 21.85 1.00 24.85 |
| MOTA | 15299 15300 | CG CD1 | | 2280 2280 | | -27.416 | 57.743 | 1.00 25.93 |
| MOTA | 15300 | CD1 | LEU | 2280 | | -27.745 | 55.278 | 1.00 25.33 |
| MOTA MOTA | 15301 | CD2 | LEU | 2280 | | -27.743 | 55.895 | 1.00 23.21 |
| ATOM | 15302 | 0 | LEU - | 2280 | | -27.842 | 56.968 | 1.00 20.23 |
| ATOM | 15303 | N | GLU | 2281 | | -28.364 | 54.783 | 1.00 20.33 |
| ATOM | 15305 | CA | GLU | 2281 | | -29.023 | 54.747 | 1.00 22.59 |
| ATOM | 15306 | CB | GLU | 2281 | | -28.328 | 53.713 | 1.00 24.29 |
| ATOM | 15307 | CG | GLU | 2281 | | -29.028 | 53.428 | 1.00 25.86 |
| ATOM | 15308 | CD | GLU | 2281 | | -28.177 | 52.592 | 1.00 28.07 |
| ATOM | 15309 | | GLU | 2281 | | -27.208 | 51.960 | 1.00 27.88 |
| MOTA | 15310 | | GLU | 2281 | 20.247 | -28.486 | 52.555 | 1.00 30.09 |
| ATOM | 15311 | С | GLU | 2281 | 24.708 | -30.513 | 54.437 | 1.00 23.66 |
| MOTA | 15312 | 0 | GLU | 2281 | 25.362 | -30.918 | 53.476 | 1.00 24.09 |
| ATOM | 15313 | N | CYS | 2282 | 24.050 | -31.316 | 55.271 | 1.00 24.83 |
| ATOM | 15314 | CA | CYS | 2282 | 24.006 | -32.764 | 55.119 | 1.00 26.77 |
| MOTA | 15315 | CB | CYS | 2282 | 22.988 | -33.136 | 54.048 | 1.00 27.38 |
| MOTA | 15316 | SG | CYS | 2282 | 21.317 | -32.574 | 54.459 | 1.00 27.22 |
| MOTA | 15317 | С | CYS | 2282 | 25.354 | -33.389 | 54.802 | 1.00 29.00 |
| ATOM | 15318 | О | CYS | 2282 | 25.623 | -33.800 | 53.670 | 1.00 28.72 |
| MOTA | 15319 | N | VAL | 2283 | 26.193 | -33.459 | 55.826 | 1.00 29.47 |
| MOTA | 15320 | CA | VAL | 2283 | | -34.025 | 55.702 | 1.00 32.15 |
| ATOM | 15321 | CB | VAL | 2283 | | 32.892 | 55.597 | 1.00 32.80 |
| ATOM | 15322 | | VAL | 2283 | | -31.988 | 56.812 | 1.00 34.08 |
| ATOM | 15323 | CG2 | VAL | 2283 | | -33.473 | 55.474 | 1.00 36.16 |
| MOTA | 15324 | C | VAL | 2283 | | -34.866 -34.529 | 56.946 58.035 | 1.00 31.72 1.00 33.06 |
| MOTA | 15325 | 0 | VAL | 2283 | | -35.986 | 56.799 | 1.00 33.00 |
| MOTA | 15326 15327 | N CD | PRO PRO | 2284 | | -36.504 | 55.614 | 1.00 31.82 |
| ATOM | 15327 | CA | PRO | 2284 | | -36.818 | 57.970 | 1.00 31.61 |
| ATOM | 15329 | CB | PRO | 2284 | | -37.866 | 57.430 | 1.00 31.74 |
| ATOM | 15330 | CG | PRO | 2284 | | -37.187 | 56.241 | 1.00 34.69 |
| ATOM | 15331 | С | PRO | 2284 | | -36.005 | 59.120 | 1.00 31.47 |
| ATOM | 15332 | Ō | PRO | 2284 | | -35.155 | | 1.00 30.70 |
| MOTA | 15333 | N | VAL | 2285 | 28.865 | -36.263 | 60.322 | 1.00 32.63 |
| ATOM | 15334 | CA | VAL | 2285 | 29.316 | -35.561 | 61.514 | 1.00 33.69 |
| MOTA | 15335 | CB | VAL | 2285 | 28.795 | -36.249 | 62.793 | 1.00 34.08 |
| MOTA | 15336 | CG1 | VAL | 2285 | 29.136 | -35.407 | 64.007 | 1.00 34.06 |
| MOTA | 15337 | CG2 | VAL | 2285 | | -36.469 | 62.695 | 1.00 35.22 |
| MOTA | 15338 | С | VAL | 2285 | | -35.506 | 61.583 | 1.00 33.95 |
| MOTA | 15339 | 0 | VAL | 2285 | | -34.488 | 61.970 | 1.00 32.97 |
| ATOM | 15340 | N | GLU | 2286 | | -36.606 | 61.200 | 1.00 35.14 |
| MOTA | 15341 | CA | GLU | 2286 | | -36.702 | 61.225 | 1.00 36.30 |
| MOTA | 15342 | CB | GLU | 2286 | | -38.045 | 60.645 | 1.00 38.87 |
| ATOM | 15343 | CG | GLU | 2286 | | -39.236 | 61.031 | 1.00 43.96 |
| ATOM | 15344 | CD OF1 | GLU | 2286 | | -39.277 -39.136 | 62.510 | 1.00 45.93 |
| ATOM ATOM | 15345 15346 | | GLU | 2286 | | -39.136 | 63.317 62.864 | 1.00 49.42 1.00 46.85 |
| MOTA MOTA | 15346 | OE2 C | GLU GLU | 2286 2286 | | -39.458 -35.579 | 60.416 | 1.00 46.83 |
| ATOM | 15347 | 0 | GLU | 2286 | | -34.868 | 60.898 | 1.00 33.02 |
| ATOM | | N | LEU | 2287 | | -35.434 | 59.176 | 1.00 34.01 |
| | 15344 | | | | | | | |
| MOTA | 15349 15350 | CA | LEU | 2287 | 33.631 | -34.406 | 58.284 | 1.00 33.45 |

| ATOM | 15352 | CG | LEU | 2287 | 33.858 -34.34 | 14 55.677 | 1.00 36.84 |
|------|-------|-----|------|------|---------------|-----------|------------|
| ATOM | 15353 | CD1 | LEU | 2287 | 33.022 -34.55 | 55 54.424 | 1.00 36.74 |
| ATOM | 15354 | CD2 | | 2287 | 34.479 -32.90 | | 1.00 38.47 |
| MOTA | 15355 | C | LEU | 2287 | 33.363 -33.02 | | 1.00 32.89 |
| ATOM | 15356 | ō | LEU | 2287 | 34.232 -32.14 | | 1.00 31.87 |
| | | N | ALA | 2288 | 32.158 -32.82 | | 1.00 32.19 |
| ATOM | 15357 | | | | | | 1.00 32.13 |
| MOTA | 15358 | CA | ALA | 2288 | 31.779 -31.54 | | |
| MOTA | 15359 | CB | ALA | 2288 | 30.367 -31.63 | | 1.00 31.39 |
| ATOM | 15360 | С | ALA | 2288 | 32.762 -31.10 | | 1.00 31.77 |
| ATOM | 15361 | 0 | ALA | 2288 | 33.092 -29.99 | 90 61.272 | 1.00 28.78 |
| ATOM | 15362 | N | LYS | 2289 | 33.219 -32.16 | 61.842 | 1.00 32.20 |
| ATOM | 15363 | CA | LYS | 2289 | 34.171 -31.96 | 62.927 | 1.00 33.72 |
| ATOM | 15364 | CB | LYS | 2289 | 34.452 -33.29 | 93 63.632 | 1.00 36.63 |
| ATOM | 15365 | CG | LYS | 2289 | 33.229 -33.94 | | 1.00 41.13 |
| ATOM | 15366 | CD | LYS | 2289 | 33.491 -35.40 | | 1.00 42.87 |
| ATOM | 15367 | CE | LYS | 2289 | 32.259 -36.04 | | 1.00 43.20 |
| ATOM | 15368 | NZ | LYS | 2289 | 32.389 -37.53 | | 1.00 42.39 |
| | | | | | | | 1.00 42.33 |
| MOTA | 15369 | C | LYS | 2289 | 35.476 -31.40 | | |
| MOTA | 15370 | 0 | LYS | 2289 | 35.966 -30.37 | | 1.00 32.46 |
| MOTA | 15371 | N | ARG | 2290 | 36.036 -32.0 | | 1.00 33.84 |
| MOTA | 15372 | CA | ARG | 2290 | 37.288 -31.65 | | 1.00 34.39 |
| ATOM | 15373 | CB | ARG | 2290 | 37.674 -32.58 | | 1.00 36.92 |
| MOTA | 15374 | CG | ARG | 2290 | 38.244 -33.92 | 22 60.066 | 1.00 39.76 |
| MOTA | 15375 | CD | ARG | 2290 | 38.859 -34.66 | 57 58.888 | 1.00 41.62 |
| ATOM | 15376 | NE | ARG | 2290 | 37.866 -35.34 | 17 58.065 | 1.00 44.41 |
| ATOM | 15377 | CZ | ARG | 2290 | 38.110 -35.84 | 10 56.853 | 1.00 45.62 |
| ATOM | 15378 | NH1 | | 2290 | 39.319 -35.72 | | 1.00 45.39 |
| ATOM | 15379 | NH2 | ARG | 2290 | 37.149 -36.46 | | |
| ATOM | 15380 | C | ARG | 2290 | 37.206 -30.22 | | 1.00 33.61 |
| | | | | 2290 | 38.051 -29.38 | | 1.00 33.01 |
| ATOM | 15381 | 0 | ARG | | | | |
| MOTA | 15382 | N | ILE | 2291 | 36.189 -29.95 | | 1.00 32.56 |
| MOTA | 15383 | CA | ILE | 2291 | 35.996 -28.62 | | 1.00 30.31 |
| MOTA | 15384 | CB | ILE | 2291 | 34.739 -28.59 | | 1.00 31.03 |
| MOTA | 15385 | CG2 | ILE | 2291 | 34.514 -27.19 | | 1.00 30.84 |
| MOTA | 15386 | CG1 | ILE | 2291 | 34.914 -29.58 | 39 56.792 | 1.00 32.84 |
| ATOM | 15387 | CD1 | ILE | 2291 | 33.694 -29.72 | 25 55.888 | 1.00 32.14 |
| MOTA | 15388 | C | ILE | 2291 | 35.860 -27.56 | 58 59.951 | 1.00 29.40 |
| MOTA | 15389 | 0 | ILE | 2291 | 36.503 -26.51 | 19 59.891 | 1.00 26.63 |
| ATOM | 15390 | N | THR | 2292 | 35.035 -27.84 | | 1.00 27.90 |
| ATOM | 15391 | CA | THR | 2292 | 34.819 -26.90 | | 1.00 28.75 |
| | 15391 | CB | THR | 2292 | 33.718 -27.40 | | 1.00 28.08 |
| ATOM | | | | | | | |
| MOTA | 15393 | OG1 | THR | 2292 | 32.489 -27.55 | | 1.00 27.32 |
| ATOM | 15394 | CG2 | THR | 2292 | 33.507 -26.41 | | 1.00 27.19 |
| MOTA | 15395 | C | THR | 2292 | 36.086 -26.63 | | 1.00 29.42 |
| MOTA | 15396 | 0 | THR | 2292 | 36.319 -25.50 | | 1.00 28.54 |
| ATOM | 15397 | N | GLU | 2293 | 36.900 -27.66 | 63.052 | 1.00 30.75 |
| MOTA | 15398 | CA | GLU | 2293 | 38.138 -27.52 | 29 63.811 | 1.00 32.20 |
| MOTA | 15399 | CB | GLU | 2293 | 38.578 -28.89 | 64.348 | 1.00 35.28 |
| ATOM | 15400 | CG | GLU | 2293 | 37.547 -29.57 | | 1.00 39.73 |
| ATOM | 15401 | CD | GLU | 2293 | 37.976 -30.95 | | 1.00 42.81 |
| ATOM | 15402 | OE1 | | 2293 | 38.390 -31.76 | | |
| ATOM | 15403 | | GLU | 2293 | 37.889 -31.25 | | 1.00 44.47 |
| | | | GLU | 2293 | 39.252 -26.92 | | 1.00 30.90 |
| ATOM | 15404 | C 1 | | | | | |
| MOTA | 15405 | • | GLU | 2293 | 40.175 -26.30 | | 1.00 31.84 |
| MOTA | 15406 | N | ALA | 2294 | 39.159 -27.10 | | 1.00 30.60 |
| MOTA | 15407 | CA | ALA | 2294 | 40.180 -26.58 | | 1.00 29.10 |
| MOTA | 15408 | СВ | ALA | 2294 | 40.190 -27.39 | | 1.00 29.45 |
| MOTA | 15409 | С | ALA | 2294 | 40.015 -25.09 | | 1.00 28.58 |
| MOTA | 15410 | 0 | ALA | 2294 | 40.996 -24.40 | | 1.00 27.98 |
| MOTA | 15411 | N | LEU. | 2295 | 38.776 -24.62 | 20 60.432 | 1.00 26.57 |
| MOTA | 15412 | CA | LEU | 2295 | 38.501 -23.22 | 25 60.111 | 1.00 26.11 |
| MOTA | 15413 | CB | LEU | 2295 | 37.178 -23.10 | 98 59.348 | 1.00 26.01 |
| MOTA | 15414 | CG | LEU | 2295 | 37.097 -23.79 | 4 57.987 | 1.00 27.63 |
| ATOM | 15415 | | LEU | 2295 | 35.761 -23.46 | | 1.00 26.37 |
| ATOM | 15416 | | LEU | 2295 | 38.242 -23.34 | | 1.00 28.50 |
| | | | | | 38.449 -22.31 | | 1.00 24.44 |
| MOTA | 15417 | С | LEU | 2295 | | | 1.00 24.44 |
| MOTA | 15418 | 0 | LEU | 2295 | | | |
| ATOM | 15419 | Ņ | ALA | 2296 | 38.953 -21.09 | | 1.00 23.89 |
| MOTA | 15420 | CA | ALA | 2296 | 38.944 -20.10 | | 1.00 23.70 |
| ATOM | 15421 | CB | ALA | 2296 | 40.053 -19.08 | | 1.00 25.57 |
| MOTA | 15422 | С | ALA | 2296 | 37.591 -19.40 | | 1.00 24.70 |
| MOTA | 15423 | 0 | ALA | 2296 | 37.079 -19.00 | | 1.00 22.57 |
| MOTA | 15424 | N | ILE | 2297 | 37.015 -19.25 | 61.009 | 1.00 23.45 |
| MOTA | 15425 | CA | ILE | 2297 | 35.715 -18.60 | 01 60.877 | 1.00 23.32 |
| ATOM | 15426 | СВ | ILE | 2297 | 35.407 -18.22 | | 1.00 22.51 |
| MOTA | 15427 | CG2 | ILE | 2297 | 36.401 -17.19 | | 1.00 23.31 |
| ATOM | 15428 | CG1 | ILE | 2297 | 35.410 -19.48 | | 1.00 22.06 |
| | | | | | | | == |

| ATOM | 15429 | CD1 | ILE | 2297 | 34.938 -19.252 | 57.130 | 1.00 23.01 |
|------|-------|-------|-----|------|----------------|--------|------------|
| ATOM | 15430 | C | ILE | 2297 | 34.625 -19.553 | 61.354 | 1.00 21.65 |
| | 15431 | | ILE | 2297 | 34.782 -20.768 | 61.288 | 1.00 22.46 |
| ATOM | | 0 | | | | | |
| MOTA | 15432 | N | PRO | 2298 | 33.499 -19.009 | 61.836 | 1.00 22.06 |
| ATOM | 15433 | CD | PRO | 2298 | 33.188 -17.587 | 62.064 | 1.00 22.11 |
| MOTA | 15434 | CA | PRO | 2298 | 32.417 -19.873 | 62.312 | 1.00 20.85 |
| MOTA | 15435 | CB | PRO | 2298 | 31.437 -18.884 | 62.942 | 1.00 21.35 |
| MOTA | 15436 | CG | PRO | 2298 | 31.698 -17.610 | 62.208 | 1.00 24.05 |
| ATOM | 15437 | C | PRO | 2298 | 31.793 -20.728 | 61.213 | 1.00 22.19 |
| | 15438 | ō | PRO | 2298 | 31.678 -20.304 | 60.062 | 1.00 20.87 |
| ATOM | | | | | 31.416 -21.945 | | |
| MOTA | 15439 | N | VAL | 2299 | | 61.585 | 1.00 20.48 |
| MOTA | 15440 | CA | VAL | 2299 | 30.802 -22.899 | 60.669 | 1.00 21.54 |
| MOTA | 15441 | CB | VAL | 2299 | 31.628 -24.208 | 60.616 | 1.00 21.85 |
| MOTA | 15442 | CG1 | VAL | 2299 | 30.961 -25.227 | 59.704 | 1.00 19.09 |
| ATOM | 15443 | CG2 | VAL | 2299 | 33.035 -23.901 | 60.144 | 1.00 21.05 |
| ATOM | 15444 | С | VAL | 2299 | 29.385 -23.234 | 61.123 | 1.00 22.17 |
| ATOM | 15445 | 0 | VAL | 2299 | 29.189 -23.842 | 62.182 | 1.00 23.34 |
| ATOM | 15446 | N | ILE | 2300 | 28.402 -22.837 | 60.322 | 1.00 19.12 |
| | | CA | ILE | 2300 | 27.001 -23.099 | 60.641 | 1.00 18.65 |
| ATOM | 15447 | | | | | | |
| MOTA | 15448 | CB | ILE | 2300 | 26.087 -21.953 | 60.142 | 1.00 20.40 |
| MOTA | 15449 | CG2 | ILE | 2300 | 24.633 -22.310 | 60.397 | 1.00 19.06 |
| MOTA | 15450 | CG1 | ILE | 2300 | 26.480 -20.641 | 60.826 | 1.00 22.26 |
| ATOM | 15451 | CD1 | ILE | 2300 | 25.706 -19.424 | 60.334 | 1.00 22.74 |
| ATOM | 15452 | С | ILE | 2300 | 26.566 -24.387 | 59.966 | 1.00 18.15 |
| ATOM | 15453 | 0 | ILE | 2300 | 26.727 -24.548 | 58.755 | 1.00 18.55 |
| MOTA | 15454 | N | GLY | 2301 | 26.007 -25.305 | 60.741 | 1.00 16.44 |
| ATOM | 15455 | CA | GLY | 2301 | 25.581 -26.564 | 60.168 | 1.00 17.23 |
| | | | | | | | |
| ATOM | 15456 | С | GLY | 2301 | 24.086 -26.811 | 60.070 | 1.00 20.10 |
| MOTA | 15457 | 0 | GLY | 2301 | 23.282 -26.228 | 60.800 | 1.00 17.24 |
| MOTA | 15458 | N | ILE | 2302 | 23.727 -27.683 | 59.134 | 1.00 21.06 |
| ATOM | 15459 | CA | ILÈ | 2302 | 22.348 -28.094 | 58.899 | 1.00 23.05 |
| MOTA | 15460 | CB | ILE | 2302 | 21.621 -27.163 | 57.872 | 1.00 26.00 |
| MOTA | 15461 | · CG2 | ILE | 2302 | 22.500 -26.896 | 56.653 | 1.00 27.12 |
| ATOM | 15462 | CG1 | ILE | 2302 | 20.295 -27.790 | 57.452 | 1.00 27.76 |
| ATOM | 15463 | CD1 | ILE | 2302 | 19.321 -27.937 | 58.577 | 1.00 31.67 |
| | | | | | 22.458 -29.517 | | 1.00 31.07 |
| ATOM | 15464 | C | ILE | 2302 | | 58.358 | |
| MOTA | 15465 | 0 | ILE | 2302 | 22.847 -29.730 | 57.211 | 1.00 23.36 |
| ATOM | 15466 | N | GLY | 2303 | 22.136 -30.493 | 59.200 | 1.00 24.09 |
| MOTA | 15467 | CA | GLY | 2303 | 22.254 -31.882 | 58.791 | 1.00 24.67 |
| ATOM | 15468 | С | GLY | 2303 | 23.715 -32.308 | 58.862 | 1.00 26.55 |
| ATOM | 15469 | 0 | GLY | 2303 | 24.149 -33.218 | 58.152 | 1.00 25.82 |
| MOTA | 15470 | N | ALA | 2304 | 24.472 -31.640 | 59.731 | 1.00 26.01 |
| ATOM | 15471 | CA | ALA | 2304 | 25.895 -31.923 | 59.910 | 1.00 26.83 |
| ATOM | 15472 | CB | ALA | 2304 | 26.721 -30.726 | 59.447 | 1.00 26.51 |
| | | | | | | 61.357 | |
| MOTA | 15473 | C | ALA | 2304 | 26.247 -32.261 | | |
| MOTA | 15474 | 0 | ALA | 2304 | 27.424 -32.321 | 61.721 | 1.00 27.78 |
| MOTA | 15475 | N | GLY | 2305 | 25.227 -32.470 | 62.184 | 1.00 29.32 |
| ATOM | 15476 | CA | GLY | 2305 | 25.465 -32.796 | 63.580 | 1.00 29.51 |
| ATOM | 15477 | С | GLY | 2305 | 25.569 -31.564 | 64.459 | 1.00 29.45 |
| ATOM | 15478 | 0 | GLY | 2305 | 25.325 -30.447 | 63.998 | 1.00 29.69 |
| ATOM | 15479 | N | ASN | 2306 | 25.934 -31.766 | 65.725 | 1.00 27.86 |
| ATOM | 15480 | CA | ASN | 2306 | 26.062 -30.663 | 66.672 | 1.00 27.30 |
| ATOM | 15481 | СВ | ASN | 2306 | 25.404 -31.029 | 68.014 | 1.00 26.47 |
| ATOM | 15482 | CG | ASN | 2306 | 26.124 -32.165 | 68.750 | 1.00 20.47 |
| | | | | | 25.801 -32.469 | 69.902 | 1.00 29.23 |
| ATOM | 15483 | | ASN | 2306 | | | |
| ATOM | 15484 | | ASN | 2306 | 27.090 -32.791 | 68.093 | 1.00 24.10 |
| MOTA | 15485 | С | ASN | 2306 | 27.508 -30.240 | 66.915 | 1.00 27.30 |
| MOTA | 15486 | 0 | ASN | 2306 | 27.801 -29.558 | 67.896 | 1.00 26.84 |
| MOTA | 15487 | N | VAL | 2307 | 28.406 -30.632 | 66.014 | 1.00 27.99 |
| ATOM | 15488 | CA | VAL | 2307 | 29.822 -30.302 | 66.150 | 1.00 27.99 |
| ATOM | 15489 | CB | VAL | 2307 | 30.706 -31.377 | 65.491 | 1.00 29.98 |
| ATOM | 15490 | | VAL | 2307 | 32.168 -31.134 | 65.843 | 1.00 32.46 |
| ATOM | 15491 | | VAL | 2307 | 30.272 -32.762 | 65.947 | 1.00 29.99 |
| | | C | VAL | 2307 | 30.168 -28.950 | 65.533 | 1.00 26.89 |
| ATOM | 15492 | | | | | | 1.00 25.00 |
| ATOM | 15493 | 0 | VAL | 2307 | 31.257 -28.414 | 65.756 | |
| ATOM | 15494 | N | THR | 2308 | 29.241 -28.402 | 64.753 | 1.00 25.39 |
| ATOM | 15495 | CA | THR | 2308 | 29.465 -27.113 | 64.116 | 1.00 24.44 |
| MOTA | 15496 | CB | THR | 2308 | 28.486 -26.890 | 62.930 | 1.00 24.99 |
| MOTA | 15497 | OG1 | THR | 2308 | 27.134 -27.038 | 63.384 | 1.00 23.48 |
| ATOM | 15498 | CG2 | THR | 2308 | 28.758 -27.897 | 61.815 | 1.00 23.59 |
| ATOM | 15499 | C | THR | 2308 | 29.293 -25.990 | 65.132 | 1.00 23.65 |
| ATOM | 15500 | ō | THR | 2308 | 28.656 -26.169 | 66.167 | 1.00 25.62 |
| ATOM | 15501 | N | ASP | 2309 | 29.871 -24.834 | 64.834 | 1.00 23.25 |
| ATOM | 15501 | | | | 29.785 -23.684 | 65.726 | 1.00 23.23 |
| | | CA | ASP | 2309 | | | |
| ATOM | 15503 | CB | ASP | 2309 | 30.642 -22.546 | 65.189 | 1.00 22.91 |
| ATOM | 15504 | CG | ASP | 2309 | 32.098 -22.940 | 65.042 | 1.00 25.32 |
| MOTA | 15505 | OD1 | ASP | 2309 | 32.722 -23.288 | 66.070 | 1.00 21.88 |
| | | | | | | | |

| ATOM | 15506 | OD2 | ASP | 2309 | 32.609 | -22.900 | 63.904 | 1.00 22.96 |
|--------|-------|-----|-----|------|--------|---------|--------|------------|
| ATOM | 15507 | С | ASP | 2309 | | -23.206 | 65.883 | 1.00 22.86 |
| ATOM | 15508 | ō | ASP | 2309 | | -22.793 | 66.966 | 1.00 23.77 |
| ATOM | 15509 | N | GLY | 2310 | | -23.257 | 64.798 | 1.00 22.07 |
| ATOM | 15510 | CA | GLY | 2310 | | -22.814 | 64.857 | 1.00 21.62 |
| ATOM | 15511 | C | GLY | 2310 | | -23.769 | 64.136 | 1.00 20.15 |
| ATOM | 15512 | Ö | GLY | 2310 | | -24.742 | 63.533 | 1.00 19.40 |
| | 15513 | N | GLN | 2311 | | -23.487 | 64.190 | 1.00 21.21 |
| MOTA | | | | 2311 | | -24.332 | 63.541 | 1.00 21.21 |
| MOTA | 15514 | CA | GLN | | | -24.332 | 64.592 | 1.00 20.52 |
| ATOM | 15515 | CB | GLN | 2311 | | | | |
| MOTA | 15516 | CG | GLN | 2311 | | -26.179 | 65.329 | 1.00 22.52 |
| ATOM | 15517 | CD | GLN | 2311 | | -27.243 | 64.390 | 1.00 21.75 |
| MOTA | 15518 | | GLN | 2311 | | -27.687 | 63.474 | 1.00 21.80 |
| MOTA | 15519 | | GLN | 2311 | | -27.666 | 64.623 | 1.00 21.19 |
| MOTA | 15520 | С | GLN | 2311 | | -23.485 | 62.736 | 1.00 20.67 |
| MOTA | 15521 | 0 | GLN | 2311 | | -22.328 | 63.071 | 1.00 17.41 |
| MOTA | 15522 | N | ILE | 2312 | | -24.060 | 61.676 | 1.00 22.09 |
| MOTA | 15523 | CA | ILE | 2312 | | -23.343 | 60.872 | 1.00 24.89 |
| MOTA | 15524 | CB | ILE | 2312 | 21.110 | -22.706 | 59.606 | 1.00 25.72 |
| ATOM | 15525 | CG2 | ILE | 2312 | 21.564 | -23.786 | 58.635 | 1.00 26.02 |
| ATOM | 15526 | CG1 | ILE | 2312 | 20.100 | -21.773 | 58.932 | 1.00 27.58 |
| ATOM | 15527 | CD1 | ILE | 2312 | 20.741 | -20.666 | 58.103 | 1.00 29.83 |
| ATOM | 15528 | С | ILE | 2312 | 19.342 | -24.292 | 60.477 | 1.00 27.16 |
| ATOM | 15529 | 0 | ILE | 2312 | 19.570 | -25.481 | 60.251 | 1.00 28.46 |
| ATOM | 15530 | N | LEU | 2313 | 18.120 | -23.774 | 60.419 | 1.00 27.96 |
| ATOM | 15531 | CA | LEU | 2313 | 16.981 | -24.604 | 60.058 | 1.00 29.89 |
| ATOM | 15532 | СВ | LEU | 2313 | | -25.308 | 61.299 | 1.00 32.34 |
| ATOM | 15533 | CG | LEU | 2313 | | -26.791 | 61.172 | 1.00 36.07 |
| ATOM | 15534 | | LEU | 2313 | | -27.236 | 62.479 | 1.00 36.26 |
| ATOM | 15535 | | LEU | 2313 | | -27.027 | 60.000 | 1.00 35.23 |
| ATOM | 15536 | C | LEU | 2313 | | -23.765 | 59.434 | 1.00 29.08 |
| ATOM | 15537 | Ö | LEU | 2313 | | -22.578 | 59.735 | 1.00 26.94 |
| ATOM | 15538 | N | | 2314 | | -24.386 | 58.558 | 1.00 28.13 |
| | | | VAL | | | -23.699 | 57.902 | 1.00 26.96 |
| MOTA | 15539 | CA | VAL | 2314 | | -23.655 | 56.647 | 1.00 28.27 |
| ATOM | 15540 | CB | VAL | 2314 | | | | |
| ATOM | 15541 | | VAL | 2314 | | -23.692 | 55.999 | 1.00 28.30 |
| MOTA | 15542 | CG2 | | 2314 | | -24.638 | 55.666 | 1.00 28.58 |
| ATOM | 15543 | C | VAL | 2314 | | -23.628 | 58.899 | 1.00 25.72 |
| MOTA | 15544 | 0 | VAL | 2314 | | -24.654 | 59.350 | 1.00 25.30 |
| ATOM | 15545 | N | MET | 2315 | | -22.411 | 59.249 | 1.00 25.28 |
| MOTA | 15546 | CA | MET | 2315 | | -22.196 | 60.205 | 1.00 22.98 |
| MOTA | 15547 | CB | MET | 2315 | | -20.711 | 60.278 | 1.00 20.69 |
| ATOM | 15548 | CG | MET | 2315 | | -20.145 | 58.960 | 1.00 20.27 |
| ATOM | 15549 | SD | MET | 2315 | | -18.854 | 59.197 | 1.00 19.44 |
| ATOM | 15550 | CE | MET | 2315 | | -19.873 | 59.416 | 1.00 17.93 |
| ATOM | 15551 | С | MET | 2315 | | -22.996 | 59.876 | 1.00 22.84 |
| MOTA | 15552 | 0 | MET | 2315 | 9.407 | -23.463 | 60.776 | 1.00 24.09 |
| MOTA | 15553 | N | HIS | 2316 | 9.807 | -23.162 | 58.591 | 1.00 23.24 |
| ATOM | 15554 | CA | HIS | 2316 | 8.616 | -23.903 | 58.180 | 1.00 22.87 |
| ATOM | 15555 | CB | HIS | 2316 | 8.445 | -23.796 | 56.662 | 1.00 21.29 |
| ATOM | 15556 | CG | HIS | 2316 | 7.970 | -22.449 | 56.216 | 1.00 20.22 |
| ATOM | 15557 | CD2 | HIS | 2316 | 8.651 | -21.318 | 55.913 | 1.00 17.37 |
| MOTA | 15558 | ND1 | HIS | 2316 | 6.633 | -22.120 | 56.152 | 1.00 20.75 |
| ATOM · | 15559 | CE1 | HIS | 2316 | 6.511 | -20.844 | 55.833 | 1.00 20.50 |
| ATOM | 15560 | | HIS | 2316 | 7.721 | -20.333 | 55.684 | 1.00 20.64 |
| ATOM | 15561 | C | HIS | 2316 | 8.612 | -25.360 | 58.634 | 1.00 24.41 |
| ATOM | 15562 | 0 | HIS | 2316 | 7.551 | -25.965 | 58.787 | 1.00 23.54 |
| ATOM | 15563 | N | ASP | 2317 | 9.790 | -25.936 | 58.845 | 1.00 25.53 |
| ATOM | 15564 | CA | ASP | 2317 | | -27.313 | 59.330 | 1.00 27.90 |
| ATOM | 15565 | CB | ASP | 2317 | | -28.029 | 58.813 | 1.00 31.10 |
| ATOM | 15566 | CG | ASP | 2317 | 10.984 | -28.436 | 57.358 | 1.00 32.92 |
| ATOM | 15567 | | ASP | 2317 | | -29.002 | 56.979 | 1.00 36.68 |
| MOTA | 15568 | | ASP | 2317 | | -28.205 | 56.598 | 1.00 35.40 |
| ATOM | 15569 | C | ASP | 2317 | | -27.291 | 60.857 | 1.00 27.46 |
| ATOM | 15570 | 0 | ASP | 2317 | | -28.140 | 61.512 | 1.00 28.41 |
| ATOM | 15571 | N | ALA | 2318 | | -26.304 | 61.410 | 1.00 28.19 |
| MOTA | 15572 | CA | ALA | 2318 | | -26.154 | 62.853 | 1.00 29.17 |
| ATOM | 15573 | CB | ALA | 2318 | | -24.946 | 63.167 | 1.00 31.06 |
| . ATOM | 15574 | СБ | ALA | 2318 | | -26.025 | 63.553 | 1.00 31.00 |
| ATOM | 15575 | 0 | ALA | 2318 | | -26.371 | 64.727 | 1.00 30.52 |
| | | | | 2319 | | -25.526 | 62.834 | 1.00 30.39 |
| ATOM | 15576 | N | PHE | | | -25.357 | 63.416 | 1.00 29.73 |
| ATOM | 15577 | CA | PHE | 2319 | | | | 1.00 29.63 |
| ATOM | 15578 | CB | PHE | 2319 | | -23.917 | 63.234 | |
| ATOM | 15579 | CG | PHE | 2319 | | -22.886 | 63.711 | 1.00 31.82 |
| ATOM | 15580 | | PHE | 2319 | | -23.020 | 64.950 | 1.00 32.14 |
| ATOM | 15581 | | PHE | 2319 | | -21.778 | 62.928 | 1.00 32.09 |
| MOTA | 15582 | CEI | PHE | 2319 | 9.056 | -22.067 | 65.398 | 1.00 32.92 |
| | | | | | | | | |

| ATOM | 15583 | CE2 | PHE | 2319 | 8.731 | -20.818 | 63.366 | 1.00 | 32.42 |
|------|-------|-----|-----|------|--------|---------|---------|------|-------|
| ATOM | 15584 | CZ | PHE | 2319 | 9.347 | -20.963 | 64.606 | 1.00 | 33.77 |
| ATOM | 15585 | C | PHE | 2319 | | -26.318 | 62.818 | | 28.48 |
| ATOM | 15586 | 0 | PHE | 2319 | | -26.115 | 62.941 | 1.00 | 29.39 |
| MOTA | 15587 | N | GLY | 2320 | | -27.368 | 62.175 | | 30.40 |
| ATOM | 15588 | CA | GLY | 2320 | | -28.357 | 61.573 | | 29.32 |
| MOTA | 15589 | C | GLY | 2320 | | -27.800 | 60.597 | | 28.92 |
| | 15590 | | | 2320 | | -28.410 | 60.380 | | 28.53 |
| MOTA | | 0 | GLY | | | -26.410 | 60.003 | | 28.40 |
| MOTA | 15591 | N | ILE | 2321 | | | | | |
| MOTA | 15592 | CA | ILE | 2321 | | -26.029 | 59.047 | | 28.56 |
| ATOM | 15593 | CB | ILE | 2321 | 4.425 | -24.573 | 58.729 | | 26.93 |
| ATOM | 15594 | CG2 | ILE | 2321 | 3.532 | -23.991 | 57.646 | | 28.95 |
| MOTA | 15595 | CG1 | ILE | 2321 | | -23.721 | 60.001 | | 27.13 |
| MOTA | 15596 | CD1 | ILE | 2321 | | -22.326 | 59.854 | | 23.13 |
| MOTA | 15597 | С | ILE | 2321 | 3.946 | -26.823 | 57.746 | | 30.05 |
| MOTA | 15598 | 0 | ILE | 2321 | | -27.052 | 57.190 | | 28.53 |
| MOTA | 15599 | N | THR | 2322 | 5.106 | -27.249 | 57.264 | | 32.75 |
| MOTA | 15600 | CA | THR | 2322 | 5.163 | -28.000 | 56.021 | 1.00 | 37.43 |
| MOTA | 15601 | CB | THR | 2322 | 6.567 | -27.946 | 55.417 | 1.00 | 38.04 |
| MOTA | 15602 | OG1 | THR | 2322 | 7.450 | -28.764 | 56.190 | 1.00 | 41.53 |
| MOTA | 15603 | CG2 | THR | 2322 | 7.084 | -26.520 | 55.431 | 1.00 | 36.66 |
| ATOM | 15604 | С | THR | 2322 | 4.775 | -29.454 | 56.242 | 1.00 | 40.21 |
| ATOM | 15605 | 0 | THR | 2322 | | -30.112 | 57.143 | 1.00 | 40.84 |
| ATOM | 15606 | N | GLY | 2323 | 3.853 | -29.942 | 55.415 | | 43.61 |
| ATOM | 15607 | CA | GLY | 2323 | | -31.320 | 55.509 | | 48.35 |
| ATOM | 15608 | C | GLY | 2323 | | -31.967 | 56.868 | | 51.33 |
| ATOM | 15609 | 0 | GLY | 2323 | | -31.368 | 57.903 | | 51.84 |
| ATOM | 15610 | N | GLY | 2324 | | -33.196 | 56.867 | | 53.18 |
| | | | | | | -33.100 | 58.116 | | 54.96 |
| ATOM | 15611 | CA | GLY | 2324 | 5.535 | | 58.065 | | 56.02 |
| ATOM | 15612 | С | GLY | 2324 | | -34.783 | | | |
| MOTA | 15613 | 0 | GLY | 2324 | | -35.358 | 59.076 | 1.00 | |
| MOTA | 15614 | N | HIS | 2325 | 6.132 | -34.889 | 56.884 | 1.00 | |
| MOTA | 15615 | CA | HIS | 2325 | 7.322 | -35.710 | 56.701 | 1.00 | 56.49 |
| ATOM | 15616 | CB | HIS | 2325 | 7.148 | -36.604 | 55.475 | | 58.75 |
| MOTA | 15617 | CG | HIS | 2325 | | -37.532 | 55.571 | 1.00 | 61.46 |
| MOTA | 15618 | | HIS | 2325 | 4.882 | -37.670 | 54.788 | | 62.32 |
| MOTA | 15619 | ND1 | HIS | 2325 | 5.852 | -38.467 | 56.576 | | 62.35 |
| MOTA | 15620 | CE1 | HIS | 2325 | | -39.141 | 56.408 | | 63.14 |
| MOTA | 15621 | NE2 | HIS | 2325 | 4.121 | -38.677 | 55.330 | 1.00 | |
| MOTA | 15622 | С | HIS | 2325 | | -34.852 | 56.543 | | 55.31 |
| MOTA | 15623 | 0 | HIS | 2325 | 9.174 | -34.805 | 55.470 | 1.00 | 55.03 |
| ATOM | 15624 | N | ILE | 2326 | 8.959 | -34.177 | 57.622 | 1.00 | 53.27 |
| MOTA | 15625 | CA | ILE | 2326 | 10.137 | -33.318 | 57.608 | 1.00 | 50.77 |
| MOTA | 15626 | CB | ILE | 2326 | 10.230 | -32.483 | 58.898 | 1.00 | 50.89 |
| MOTA | 15627 | CG2 | ILE | 2326 | 8.991 | -31.612 | 59.043 | 1.00 | 50.89 |
| MOTA | 15628 | CG1 | ILE | 2326 | 10.380 | -33.408 | 60.107 | 1.00 | 51.06 |
| ATOM | 15629 | CD1 | ILE | 2326 | | -32.672 | 61.410 | 1.00 | 50.63 |
| ATOM | 15630 | С | ILE | 2326 | 11.408 | -34.151 | 57.473 | | 48.48 |
| ATOM | 15631 | ō | ILE | 2326 | | -35.356 | | | 48.12 |
| ATOM | 15632 | N | PRO | 2327 | 12.523 | -33.517 | 57.076 | 1.00 | 46.61 |
| ATOM | 15633 | CD | PRO | 2327 | 12.695 | -32.092 | 56.746 | 1.00 | 46.53 |
| ATOM | 15634 | CA | PRO | 2327 | | -34.247 | 56.923 | | 45.07 |
| ATOM | 15635 | CB | PRO | 2327 | | -33.205 | 56.296 | | 45.91 |
| ATOM | 15636 | CG | PRO | 2327 | | -31.918 | 56.854 | 1.00 | 46.83 |
| | | | PRO | 2327 | | -34.796 | 58.245 | | 43.14 |
| ATOM | 15637 | C | | | 13.982 | -34.292 | 59.318 | 1.00 | |
| ATOM | 15638 | 0 | PRO | 2327 | 15.144 | -35.833 | 58.163 | 1.00 | 41.21 |
| ATOM | 15639 | N | LYS | 2328 | | | | | |
| ATOM | 15640 | CA | LYS | 2328 | 15.716 | -36.455 | 59.354 | | 38.78 |
| ATOM | 15641 | CB | LYS | 2328 | | -37.692 | 58.967 | 1.00 | 41.48 |
| MOTA | 15642 | CG | LYS | 2328 | | -38.917 | 58.617 | | 45.03 |
| MOTA | 15643 | CD | LYS | 2328 | | -38.644 | 57.447 | | 47.19 |
| MOTA | 15644 | CE | LYS | 2328 | | -39.779 | 57.245 | | 48.48 |
| MOTA | 15645 | NZ | LYS | 2328 | 12.793 | -39.463 | 56.165 | | 49.27 |
| MOTA | 15646 | С | LYS | 2328 | 16.583 | -35.513 | 60.181 | | 35.61 |
| MOTA | 15647 | 0 | LYS | 2328 | 16.774 | -35.732 | 61.376 | | 34.87 |
| MOTA | 15648 | N | PHE | 2329 | 17.102 | -34.463 | 59.553 | | 31.28 |
| MOTA | 15649 | CA | PHE | 2329 | 17.955 | -33.514 | 60.262 | | 28.57 |
| MOTA | 15650 | CB | PHE | 2329 | 19.028 | -32.967 | 59.315 | 1.00 | 28.07 |
| MOTA | 15651 | CG | PHE | 2329 | 18.480 | -32.290 | 58.089 | 1.00 | 29.05 |
| MOTA | 15652 | CD1 | | 2329 | 17.954 | -31.004 | 58.157 | 1.00 | 28.21 |
| MOTA | 15653 | | PHE | 2329 | 18.506 | -32.935 | 56.857 | 1.00 | 29.00 |
| MOTA | 15654 | CE1 | | 2329 | 17.470 | -30.367 | 57.011 | | 28.14 |
| MOTA | 15655 | CE2 | PHE | 2329 | | -32.309 | 55.708 | | 28.09 |
| MOTA | 15656 | CZ | PHE | 2329 | | -31.023 | 55.785 | | 29.29 |
| ATOM | 15657 | c | PHE | 2329 | | -32.365 | 60.896 | | 26.22 |
| ATOM | 15658 | ō | PHE | 2329 | | -31.568 | 61.649 | | 24.18 |
| ATOM | 15659 | N | ALA | 2330 | | -32.288 | 60.597 | | 26.36 |
| | | • | | | | | · · · · | | |

| ATOM | 15660 | CA | ALA | 2330 | 15.051 -31.225 | 61.133 | 1.00 25.12 |
|---|---|---|---|--|--|--|--|
| ATOM | 15661 | CB | ALA | 2330 | 14.109 -30.721 | 60.048 | 1.00 24.79 |
| ATOM | 15662 | C | ALA | 2330 | 14.250 -31.701 | | 1.00 25.45 |
| ATOM | 15663 | ō | ALA | 2330 | 14.066 -32.900 | | 1.00 26.65 |
| | | N | LYS | 2331 | 13.761 -30.753 | | 1.00 25.57 |
| ATOM | 15664 | | | | 12.966 -31.068 | | 1.00 25.38 |
| ATOM | 15665 | CA | LYS | 2331 | | | |
| MOTA | 15666 | CB | LYS | 2331 | 13.861 -31.093 | | 1.00 26.54 |
| MOTA | 15667 | CG | LYS | 2331 | 13.128 -31.323 | 66.853 | 1.00 27.14 |
| ATOM | 15668 | CD | LYS | 2331 | 14.114 -31.423 | 68.013 | 1.00 27.67 |
| ATOM | 15669 | CE | LYS | 2331 | 13.404 -31.585 | 69.352 | 1.00 28.98 |
| ATOM | 15670 | NZ | LYS | 2331 | 14.389 -31.782 | 70.465 | 1.00 25.48 |
| ATOM | 15671 | C | LYS | 2331 | 11.845 -30.051 | | 1.00 24.96 |
| ATOM | 15672 | ō | LYS | 2331 | 12.060 -28.842 | | 1.00 23.50 |
| | | | | 2332 | 10.647 -30.553 | | 1.00 24.26 |
| ATOM | 15673 | N | ASN | | | | 1.00 24.20 |
| ATOM | 15674 | CA | ASN | 2332 | 9.488 -29.697 | | |
| MOTA | 15675 | CB | ASN | 2332 | 8.197 -30.456 | | 1.00 23.26 |
| MOTA | 15676 | CG | ASN | 2332 | 6.941 -29.655 | | 1.00 22.69 |
| MOTA | 15677 | OD1 | ASN | 2332 | 7.009 -28.540 | 65.474 | 1.00 23.56 |
| MOTA | 15678 | ND2 | ASN | 2332 | 5.788 -30.226 | 64.641 | 1.00 23.07 |
| ATOM | 15679 | С | ASN | 2332 | 9.469 -29.286 | 66.446 | 1.00 23.54 |
| ATOM | 15680 | 0 | ASN | 2332 | 9.098 -30.076 | 67.311 | 1.00 25.07 |
| ATOM | 15681 | N | PHE | 2333 | 9.874 -28.054 | | 1.00 25.71 |
| ATOM | 15682 | CA | PHE | 2333 | 9.894 -27.567 | | 1.00 26.02 |
| | 15683 | CB | PHE | 2333 | 10.884 -26.411 | | 1.00 27.67 |
| ATOM | | | | | | | 1.00 27.07 |
| ATOM | 15684 | CG | PHE | 2333 | 12.317 -26.826 | | |
| ATOM | 15685 | | PHE | 2333 | 12.885 -26.981 | | 1.00 24.93 |
| MOTA | 15686 | | PHE | 2333 | 13.091 -27.086 | | 1.00 25.58 |
| MOTA | 15687 | CE1 | PHE | 2333 | 14.210 -27.392 | 66.706 | 1.00 25.54 |
| ATOM | 15688 | CE2 | PHE | 2333 | 14.416 -27.498 | 69.098 | 1.00 27.73 |
| MOTA | 15689 | CZ | PHE | 2333 | 14.972 -27.649 | 67.836 | 1.00 24.35 |
| MOTA | 15690 | С | PHE | 2333 | 8.529 -27.126 | 68.606 | 1.00 28.07 |
| ATOM | 15691 | 0 | PHE | 2333 | 8.295 -27.112 | 69.812 | 1.00 26.50 |
| MOTA | 15692 | N | LEU | 2334 | 7.633 -26.759 | | 1.00 28.99 |
| ATOM | 15693 | CA | LEU | 2334 | 6.296 -26.330 | | 1.00 30.49 |
| | | | | | 5.497 -25.820 | | 1.00 28.12 |
| ATOM | 15694 | CB | LEU | 2334 | | | |
| MOTA | 15695 | CG | LEU | 2334 | 4.023 -25.483 | | 1.00 27.45 |
| MOTA | 15696 | | LEU | 2334 | 3.933 -24.502 | | 1.00 24.55 |
| ATOM | 15697 | CD2 | LEU | 2334 | 3.363 -24.897 | | 1.00 25.02 |
| MOTA | 15698 | С | LEU | 2334 | 5.548 -27.485 | | 1.00 32.07 |
| ATOM | 15699 | 0 | LEU | 2334 | 4.865 -27.297 | | 1.00 32.09 |
| MOTA | 15700 | N | ALA | 2335 | 5.688 -28.678 | 68.177 | 1.00 35.05 |
| MOTA | 15701 | CA | ALA | 2335 | 5.030 -29.877 | 68.694 | 1.00 38.84 |
| ATOM | 15702 | CB | ALA | 2335 | 5.356 -31.072 | 67.810 | 1.00 38.92 |
| MOTA | 15703 | С | ALA | 2335 | 5.452 -30.162 | 70.130 | 1.00 41.82 |
| ATOM | 15704 | 0 | ALA | 2335 | 4.646 -30.605 | | 1.00 42.61 |
| ATOM | 15705 | N | GLU | 2336 | 6.723 -29.90 | | 1.00 45.17 |
| ATOM | 15706 | CA | GLU | 2336 | 7.273 -30.115 | | 1.00 48.42 |
| | | | | | 8.790 -29.899 | | 1.00 50.16 |
| MOTA | 15707 | CB | GLU | 2336 | | | |
| MOTA | 15708 | CG | GLU | 2336 | 9.571 -30.928 | | 1.00 52.50 |
| ATOM | 15709 | CD | GLU | 2336 | 9.730 -32.246 | | |
| ATOM | 15710 | OE1 | | 2336 | 8.701 -32.873 | | 1.00 54.49 |
| MOTA | 15711 | OE2 | GLU | 2336 | 10.888 -32.655 | 71.906 | 1.00 54.14 |
| MOTA | 15712 | C | GLU | 2336 | 6.639 -29.130 | 72.739 | 1.00 49.37 |
| MOTA | 15713 | 0 | GLU | 2336 | 6.895 -29.184 | 73.941 | 1.00 49.41 |
| MOTA | 15714 | N | THR | 2337 | 5.816 -28.228 | 72.211 | 1.00 49.87 |
| ATOM | 15715 | CA | THR | 2337 | 5.150 -27.220 | 73.026 | 1.00 49.76 |
| ATOM | 15716 | CB | THR | 2337 | 6.024 -25.946 | | 1.00 50.97 |
| ATOM | 15717 | OG1 | THR | 2337 | 5.387 -24.99 | | 1.00 52.74 |
| ATOM | 15718 | CG2 | THR | 2337 | 6.235 -25.319 | | 1.00 51.29 |
| | 15719 | | | | 3.793 -26.853 | | 1.00 48.80 |
| MOTA MOTA | | C | THR | 2337 2337 | 3.150 -27.676 | | |
| | | | | | | | |
| | 15720 | 0 | THR | | | | 1.00 48.94 |
| MOTA | 15720 15721 | O N | GLY | 2338 | 3.356 -25.619 | 72.651 | 1.00 47.93 |
| ATOM ATOM | 15720 15721 15722 | O N CA | GLY GLY | 2338 2338 | 3.356 -25.619 2.080 -25.178 | 72.651 72.114 | 1.00 47.93 1.00 45.01 |
| MOTA MOTA MOTA | 15720 15721 15722 15723 | O N CA C | GLY GLY | 2338 2338 2338 | 3.356 -25.619 2.080 -25.178 2.136 -23.730 | 72.651 72.114 71.680 | 1.00 47.93 1.00 45.01 1.00 43.22 |
| ATOM ATOM | 15720 15721 15722 15723 15724 | O N CA | GLY GLY GLY | 2338 2338 2338 2338 | 3.356 -25.619 2.080 -25.178 2.136 -23.730 1.137 -23.163 | 72.651 72.114 71.680 71.243 | 1.00 47.93 1.00 45.01 1.00 43.22 1.00 43.86 |
| MOTA MOTA MOTA | 15720 15721 15722 15723 | O N CA C | GLY GLY | 2338 2338 2338 2338 2339 | 3.356 -25.619 2.080 -25.178 2.136 -23.730 1.137 -23.163 3.317 -23.134 | 72.651 72.114 71.680 71.243 71.795 | 1.00 47.93 1.00 45.01 1.00 43.22 1.00 43.86 1.00 40.41 |
| ATOM ATOM ATOM ATOM | 15720 15721 15722 15723 15724 | O N CA C | GLY GLY GLY | 2338 2338 2338 2338 | 3.356 -25.619 2.080 -25.178 2.136 -23.730 1.137 -23.163 | 72.651 72.114 71.680 71.243 71.795 | 1.00 47.93 1.00 45.01 1.00 43.22 1.00 43.86 |
| ATOM ATOM ATOM ATOM ATOM | 15720 15721 15722 15723 15724 15725 | O N CA C O N | GLY GLY GLY GLY ASP | 2338 2338 2338 2338 2339 | 3.356 -25.619 2.080 -25.178 2.136 -23.730 1.137 -23.163 3.317 -23.134 | 72.651 72.114 71.680 71.243 71.795 71.426 | 1.00 47.93 1.00 45.01 1.00 43.22 1.00 43.86 1.00 40.41 |
| MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA | 15720 15721 15722 15723 15724 15725 15726 15727 | O N CA C O N CA CB | GLY GLY GLY GLY ASP ASP | 2338 2338 2338 2338 2339 2339 2339 | 3.356 -25.619 2.080 -25.178 2.136 -23.730 1.137 -23.163 3.317 -23.134 3.518 -21.739 | 72.651 72.114 71.680 71.243 71.795 71.426 72.696 | 1.00 47.93 1.00 45.01 1.00 43.22 1.00 43.86 1.00 40.41 1.00 38.45 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 15720 15721 15722 15723 15724 15725 15726 15727 15728 | O N CA C O N CA CB CG | GLY GLY GLY ASP ASP ASP ASP | 2338 2338 2338 2338 2339 2339 2339 2339 | 3.356 -25.619 2.080 -25.178 2.136 -23.730 1.137 -23.133 3.317 -23.134 3.518 -21.733 3.672 -20.898 3.966 -19.444 | 72.651 72.114 71.680 71.243 71.795 71.426 72.696 72.402 | 1.00 47.93 1.00 45.01 1.00 43.22 1.00 43.86 1.00 40.41 1.00 38.45 1.00 40.39 1.00 43.35 |
| MOTA ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 15720 15721 15722 15723 15724 15725 15726 15727 15728 15729 | O N CA C O N CA CB CG OD1 | GLY GLY GLY ASP ASP ASP ASP | 2338 2338 2338 2338 2339 2339 2339 2339 | 3.356 -25.619 2.080 -25.178 2.136 -23.730 1.137 -23.163 3.317 -23.134 3.518 -21.738 3.672 -20.899 3.966 -19.444 5.137 -19.123 | 72.651 72.114 71.680 71.243 71.795 71.426 72.696 72.402 72.115 | 1.00 47.93 1.00 45.01 1.00 43.22 1.00 43.86 1.00 40.41 1.00 38.45 1.00 40.39 1.00 43.35 1.00 42.97 |
| MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA | 15720 15721 15722 15723 15724 15725 15726 15727 15728 15729 15730 | O N CA C O N CA CB CG OD1 OD2 | GLY GLY GLY ASP ASP ASP ASP ASP | 2338 2338 2338 2338 2339 2339 2339 2339 | 3.356 -25.619 2.080 -25.178 2.136 -23.730 1.137 -23.163 3.317 -23.134 3.518 -21.739 3.672 -20.899 3.966 -19.444 5.137 -19.123 3.018 -18.624 | 72.651 72.114 71.680 71.243 71.795 71.426 72.696 72.402 72.115 72.448 | 1.00 47.93 1.00 45.01 1.00 43.22 1.00 43.86 1.00 40.41 1.00 38.45 1.00 40.39 1.00 43.35 1.00 42.97 1.00 45.56 |
| MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA | 15720 15721 15722 15723 15724 15725 15726 15727 15728 15729 15730 15731 | O N CA C CA CB CG OD1 OD2 C | GLY GLY GLY ASP ASP ASP ASP ASP | 2338 2338 2338 2339 2339 2339 2339 2339 | 3.356 -25.619 2.080 -25.178 2.136 -23.730 1.137 -23.163 3.317 -23.134 3.518 -21.739 3.672 -20.899 3.966 -19.444 5.137 -19.122 3.018 -18.624 4.749 -21.598 | 72.651 72.114 71.680 71.243 71.795 71.426 72.696 72.402 72.115 72.448 70.535 | 1.00 47.93 1.00 45.01 1.00 43.22 1.00 43.86 1.00 40.41 1.00 38.45 1.00 40.39 1.00 43.35 1.00 42.97 1.00 45.56 1.00 35.60 |
| MOTA ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 15720 15721 15722 15723 15724 15725 15726 15727 15728 15729 15730 15731 15732 | O N CA CB CG OD1 OD2 C | GLY GLY GLY ASP ASP ASP ASP ASP ASP ASP | 2338 2338 2338 2339 2339 2339 2339 2339 | 3.356 -25.619 2.080 -25.178 2.136 -23.730 1.137 -23.163 3.317 -23.134 3.518 -21.739 3.672 -20.899 3.966 -19.444 5.137 -19.122 3.018 -18.624 4.749 -21.598 5.797 -22.194 | 72.651 72.114 71.680 71.243 71.795 71.426 72.696 72.402 72.115 72.448 70.535 70.800 | 1.00 47.93 1.00 45.01 1.00 43.22 1.00 43.86 1.00 40.41 1.00 38.45 1.00 40.39 1.00 43.35 1.00 42.97 1.00 45.56 1.00 35.60 1.00 33.62 |
| MOTA ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 15720 15721 15722 15723 15724 15725 15726 15727 15728 15729 15730 15731 15732 15733 | O N CA CB CG OD1 OD2 C O N | GLY GLY GLY ASP ASP ASP ASP ASP ASP ASP ASP | 2338 2338 2338 2339 2339 2339 2339 2339 | 3.356 -25.619 2.080 -25.178 2.136 -23.730 1.137 -23.163 3.317 -23.134 3.518 -21.739 3.672 -20.899 3.966 -19.444 5.137 -19.122 3.018 -18.624 4.749 -21.598 5.797 -22.194 | 72.651 72.114 71.680 71.243 71.795 71.426 72.696 72.402 72.115 72.448 70.535 70.800 69.474 | 1.00 47.93 1.00 45.01 1.00 43.22 1.00 43.86 1.00 40.41 1.00 38.45 1.00 40.39 1.00 43.35 1.00 42.97 1.00 45.56 1.00 35.60 1.00 33.62 1.00 32.17 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 15720 15721 15722 15723 15724 15725 15726 15727 15728 15730 15731 15732 15733 15734 | O N CA C CB CG OD1 OD2 C O N CA | GLY GLY GLY ASP ASP ASP ASP ASP ASP ILE ILE | 2338 2338 2338 2339 2339 2339 2339 2339 | 3.356 -25.619 2.080 -25.178 2.136 -23.730 1.137 -23.163 3.317 -23.134 3.518 -21.739 3.672 -20.899 3.966 -19.444 5.137 -19.122 3.018 -18.624 4.749 -21.598 5.797 -22.194 4.618 -20.810 5.722 -20.606 | 72.651 72.114 71.680 71.243 71.426 72.696 72.402 72.115 72.448 70.535 70.800 69.474 68.540 | 1.00 47.93 1.00 45.01 1.00 43.22 1.00 43.86 1.00 40.41 1.00 38.45 1.00 40.39 1.00 43.35 1.00 42.97 1.00 45.56 1.00 35.60 1.00 33.62 1.00 32.17 1.00 29.10 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 15720 15721 15722 15723 15724 15725 15726 15727 15728 15729 15730 15731 15733 15733 15733 | O N CA C CB CG OD1 CC C C C C C C C C C C C C C C C C C | GLY GLY GLY ASP ASP ASP ASP ASP ASP ILE ILE | 2338 2338 2338 2339 2339 2339 2339 2339 | 3.356 -25.619 2.080 -25.178 2.136 -23.73 1.137 -23.163 3.317 -23.134 3.518 -21.733 3.672 -20.899 3.966 -19.444 5.137 -19.123 3.018 -18.624 4.749 -21.598 5.797 -22.194 4.618 -20.816 5.722 -20.606 5.268 -19.753 | 72.651 72.114 71.680 71.243 71.795 71.426 72.696 72.402 72.115 72.448 70.535 70.800 69.474 68.540 67.333 | 1.00 47.93 1.00 45.01 1.00 43.22 1.00 43.86 1.00 40.41 1.00 38.45 1.00 40.39 1.00 43.35 1.00 42.97 1.00 45.56 1.00 33.62 1.00 32.17 1.00 29.10 1.00 28.53 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 15720 15721 15722 15723 15724 15725 15726 15727 15728 15730 15731 15732 15733 15734 | O N CA C CB CG OD1 OD2 C O N CA | GLY GLY GLY ASP ASP ASP ASP ASP ASP ILE ILE | 2338 2338 2338 2339 2339 2339 2339 2339 | 3.356 -25.619 2.080 -25.178 2.136 -23.730 1.137 -23.163 3.317 -23.134 3.518 -21.739 3.672 -20.899 3.966 -19.444 5.137 -19.122 3.018 -18.624 4.749 -21.598 5.797 -22.194 4.618 -20.810 5.722 -20.606 | 72.651 72.114 71.680 71.243 71.795 71.426 72.696 72.402 72.115 72.448 70.535 70.800 69.474 68.540 67.333 | 1.00 47.93 1.00 45.01 1.00 43.22 1.00 43.86 1.00 40.41 1.00 38.45 1.00 40.39 1.00 43.35 1.00 42.97 1.00 45.56 1.00 35.60 1.00 33.62 1.00 32.17 1.00 29.10 |

| MOTA | 15737 | CG1 | ILE | 2340 | 4.143 -20.477 | 66.587 | 1.00 27.31 |
|--------------|----------------|------------|------------|--------------|----------------------------------|------------------|--------------------------|
| ATOM | 15738 | CD1 | ILE | 2340 | 3.507 -19.653 | 65.474 | 1.00 27.21 |
| ATOM | 15739 | С | ILE | 2340 | 6.930 -19.945 | 69.202 | 1.00 27.86 |
| ATOM | 15740 | 0 | ILE | 2340 | 8.064 -20.405 | 69.045 | 1.00 27.30 |
| ATOM | 15741 | N | ARG | 2341 | 6.693 -18.867 | 69.942 | 1.00 25.33 |
| ATOM | 15742 | CA | ARG | 2341 | 7.788 -18.180 | 70.611 | 1.00 24.52 |
| ATOM | 15743 | CB | ARG | 2341 | 7.268 -16.927 | 71.323 | 1.00 23.55 |
| ATOM | 15744 | CG | ARG | 2341 | 6.902 -15.805 | 70.349 | 1.00 24.38 |
| ATOM | 15745 | CD | ARG | 2341 | 6.378 -14.561 | 71.051 | 1.00 27.22 |
| ATOM | 15746 | NE | ARG | 2341 | 6.060 -13.502 | 70.091 | 1.00 27.15 |
| ATOM | 15747 | CZ | ARG | 2341 | 5.076 -13.577 | 69.200 | 1.00 28.36 |
| MOTA | 15748 | NH1 | ARG | 2341 | 4.308 -14.657 | 69.149 | 1.00 26.92 |
| ATOM | 15749 | NH2 | ARG | 2341 | 4.871 -12.578 | 68.354 | 1.00 27.62 |
| ATOM | 15750 | С | ARG | 2341 | 8.499 -19.116 | 71.584 | 1.00 24.05 |
| ATOM | 15751 | 0 | ARG | 2341 | 9.713 -19.030 | 71.753 | 1.00 23.07 |
| MOTA | 15752 | N | ALA | 2342 | 7.742 -20.019 | 72.202 | 1.00 23.18 |
| MOTA | 15753 | CA | ALA | 2342 | 8.307 -20.987 | 73.138 | 1.00 24.94 |
| MOTA | 15754 | CB | ALA | 2342 | 7.194 -21.728 | 73.858 | 1.00 24.89 |
| MOTA | 15755 | C | ALA | 2342 | 9.179 -21.973 | 72.367 | 1.00 24.76 |
| MOTA | 15756 | 0 | ALA | 2342 | 10.204 -22.436 | 72.865 | 1.00 25.19 |
| MOTA | 15757 | N | ALA | 2343 | 8.755 -22.291 | 71.145 | 1.00 22.90 |
| MOTA | 15758 | CA | ALA | 2343 | 9.485 -23.210 | 70.281 | 1.00 21.20 |
| MOTA | 15759 | CB | ALA | 2343 | 8.648 -23.541 | 69.049 | 1.00 23.10 |
| MOTA | 15760 | C | ALA | 2343 | 10.810 -22.574 | 69.869 | 1.00 20.25 |
| MOTA | 15761 | 0 | ALA | 2343 | 11.840 -23.246 | 69.810 | 1.00 19.96 |
| MOTA | 15762 | N | VAL | 2344 | 10.774 -21.273 | 69.586 | 1.00 20.13 |
| MOTA | 15763 | CA | VAL | 2344 | 11.964 -20.530 | 69.203 | 1.00 20.13 |
| MOTA | 15764 | CB | VAL | 2344 | 11.612 -19.069 | 68.829 | 1.00 19.76 |
| MOTA | 15765 | CG1 | | 2344 | 12.883 -18.263 | 68.605 | 1.00 21.02 |
| MOTA | 15766 | CG2 | VAL | 2344 | 10.751 -19.057 | 67.560 | 1.00 21.33 |
| MOTA | 15767 | C | VAL | 2344 | 12.983 -20.528 | 70.343 | 1.00 20.91 |
| MOTA | 15768 | 0 | VAL | 2344 | 14.186 -20.685 | 70.115 | 1.00 18.15 |
| MOTA | 15769 | N | ARG | 2345 | 12.504 -20.367 | 71.572 | 1.00 21.37 |
| ATOM | 15770 | CA | ARG | 2345 | 13.400 -20.354 | 72.721 | 1.00 23.97 |
| ATOM | 15771 | CB | ARG | 2345 | 12.664 -19.858 | 73.968 | 1.00 24.17 |
| MOTA | 15772 | CG | ARG | 2345 | 12.197 -18.414 | 73.882 | 1.00 24.76 |
| ATOM | 15773 | CD | ARG | 2345 | 11.797 -17.895 | 75.260 | 1.00 25.91 |
| MOTA | 15774 | NE | ARG | 2345 | 10.763 -18.723 | 75.872 | 1.00 27.57 |
| ATOM | 15775 | CZ | ARG | 2345 | 9.465 -18.611 | 75.617 | 1.00 28.92 |
| MOTA | 15776 | NH1 | | 2345 | 9.027 -17.698 | 74.758 | 1.00 28.97 |
| ATOM | 15777 | NH2 | | 2345 | 8.604 -19.417 | 76.218 | 1.00 30.22 |
| ATOM | 15778 | С | ARG | 2345 | 13.986 -21.742 | 72.974 | 1.00 25.12 |
| MOTA | 15779 | 0 | ARG | 2345 | 15.155 -21.870 | 73.337 | 1.00 26.08 |
| MOTA | 15780 | N | GLN | 2346 | 13.179 -22.778 | 72.772 | 1.00 24.82 |
| MOTA | 15781 | CA | GLN | 2346 | 13.649 -24.137 | 72.980 | 1.00 25.54 |
| MOTA | 15782 | CB | GLN | 2346 | 12.505 -25.133 | 72.822 | 1.00 27.18 |
| ATOM | 15783 | CG | GLN | 2346 | 12.832 -26.509 | 73.367 | 1.00 32.29 |
| ATOM | 15784 | CD | GLN | 2346 | 11.790 -27.544 | 72.996 | 1.00 35.43 |
| ATOM | 15785 | | GLN | 2346 | 10.589 -27.269 | 73.029 | 1.00 38.83 |
| MOTA | 15786 | NE2 | GLN | 2346 | 12.242 -28.746 | 72.648 | 1.00 36.41 |
| ATOM | 15787 | C | GLN | 2346 | 14.753 -24.461 | 71.974 | 1.00 25.43 |
| ATOM | 15788 | 0 | GLN | 2346 | 15.747 -25.104 | 72.309 | 1.00 24.79 |
| ATOM | 15789 | N | TYR | 2347 | 14.571 -24.008 | 70.738 | 1.00 24.34 1.00 24.09 |
| MOTA | 15790 | CA | TYR | 2347 | 15.555 -24.230 | 69.685 | |
| ATOM | 15791 | CB | TYR | 2347 | 15.043 -23.659 16.087 -23.560 | 68.358 | 1.00 24.72 |
| ATOM | 15792 | CG CD1 | TYR | 2347 | | 67.259 66.919 | 1.00 24.42 1.00 25.35 |
| ATOM ATOM | 15793 15794 | CD1 CE1 | | 2347 | 16.883 -24.656 17.814 -24.580 | 65.878 | 1.00 23.35 |
| ATOM | 15794 15795 | CD2 | | 2347 2347 | 16.248 -22.378 | 66.533 | 1.00 23.82 |
| | | CE2 | | | 17.174 -22.290 | 65.489 | 1.00 23.75 |
| ATOM ATOM | 15796 15797 | CE2 | TYR | 2347 2347 | 17.174 -22.290 | 65.169 | 1.00 24.65 |
| ATOM | 15798 | OH | TYR | 2347 | 18.864 -23.316 | 64.135 | 1.00 24.72 |
| | | | | | | 70.052 | 1.00 24.23 |
| MOTA MOTA | 15799 15800 | С 0 | TYR TYR | 2347 2347 | 16.872 -23.569 17.933 -24.175 | 69.930 | 1.00 24.13 |
| ATOM | 15801 | | MET | 2347 | 16.799 -22.320 | 70.501 | 1.00 24.26 |
| ATOM | 15801 | N CA | MET | 2348 | 17.996 -21.575 | 70.887 | 1.00 24.28 |
| ATOM | 15802 | CB | MET | 2348 | 17.606 -20.179 | 71.376 | 1.00 25.61 |
| ATOM | 15804 | CG | MET | 2348 | 17.038 -19.273 | 70.298 | 1.00 26.13 |
| ATOM | 15805 | SD | MET | 2348 | 16.196 -17.821 | 70.238 | 1.00 20.95 |
| ATOM | 15806 | CE | | 2348 | 17.540 -17.070 | 71.910 | 1.00 30.88 |
| ATOM | 15807 | CE | MET MET | 2348 | 18.748 -22.305 | 71.910 | 1.00 25.38 |
| ATOM | 15807 | 0 | MET | 2348 | 19.973 -22.437 | 71.944 | 1.00 23.38 |
| ATOM | 15809 | N | ALA | 2349 | 17.993 -22.782 | 72.973 | 1.00 25.63 |
| ATOM | 15810 | CA | ALA | 2349 | 18.546 -23.490 | 74.121 | 1.00 25.83 |
| ATOM | 15811 | CB | ALA | 2349 | 17.452 -23.694 | 75.165 | 1.00 26.84 |
| ATOM | 15812 | СВ | ALA | 2349 | 19.189 -24.832 | 73.784 | 1.00 20.84 |
| ATOM | 15813 | 0 | ALA | 2349 | 20.325 -25.094 | 74.176 | 1.00 27.32 |
| | | - | | | 20.023 20.071 | | 2 |

| MOTA | 15814 | N | GLU | 2350 | | 18.461 | -25.681 | 73.065 | 1.00 | 27.55 |
|------|-------|-----------|-----|-------|---|--------|---------|--------|------|-------|
| MOTA | 15815 | CA | GLU | 2350 | | 18.982 | -26.998 | 72.715 | | 28.05 |
| MOTA | 15816 | СВ | GLU | 2350 | | | -27.832 | 72.020 | | 27.67 |
| MOTA | 15817 | CG | GLU | 2350 | | | | 72.838 | | 30.51 |
| ATOM | 15818 | CD | GLU | 2350 | | 15.822 | -29.206 | 72.325 | | 30.48 |
| ATOM | 15819 | | GLU | 2350 | | | -29.475 | 71.108 | | 32.21 |
| ATOM | 15820 | OE2 | | 2350 | | 15.124 | -29.849 | 73.135 | | 33.22 |
| ATOM | 15821 | C | GLU | 2350 | | 20.233 | -26.937 | 71.844 | | 28.06 |
| ATOM | 15822 | ō | GLU | 2350 | | | -27.849 | 71.877 | | 26.63 |
| ATOM | 15823 | N | VAL | 2351 | | | -25.873 | 71.060 | 1.00 | |
| ATOM | 15824 | CA | VAL | 2351 | | 21.548 | -25.732 | 70.210 | | 28.48 |
| ATOM | 15825 | CB | VAL | 2351 | | | -24.605 | 69.162 | | 29.53 |
| ATOM | 15826 | | VAL | 2351 | | 22.678 | -24.341 | 68.438 | | 28.56 |
| ATOM | 15827 | CG2 | | 2351 | | | -25.003 | 68.162 | | 26.63 |
| MOTA | 15828 | C | VAL | 2351 | | | -25.406 | 71.091 | | 30.61 |
| ATOM | 15829 | 0 | VAL | 2351 | | | -26.061 | 71.091 | | 29.24 |
| ATOM | 15830 | N | GLU | 2352 | | | -24.404 | 71.951 | | 31.03 |
| ATOM | 15831 | CA | GLU | 2352 | | 23.676 | -23.997 | 72.840 | | 33.56 |
| | 15832 | CB | GLU | 2352 | | | -23.337 | 73.681 | | 34.00 |
| ATOM | | | | | | | | | | |
| ATOM | 15833 | CG | GLU | 2352 | | | -22.236 | 74.554 | | 38.30 |
| ATOM | 15834 | CD CD1 | GLU | 2352 | | 23.923 | -21.011 | 75.328 | | 40.92 |
| MOTA | 15835 | OE1 | GLU | 2352 | | | -20.485 | 76.109 | | 42.56 |
| ATOM | 15836 | OE2 | GLU | 2352 | | | -20.571 | 75.159 | | 42.53 |
| ATOM | 15837 | C | GLU | 2352 | | 24.108 | -25.137 | 73.760 | | 34.18 |
| MOTA | 15838 | 0 | GLU | 2352 | | | -25.266 | 74.090 | | 34.72 |
| MOTA | 15839 | N | SER | 2353 | | | -25.963 | 74.166 | | 33.74 |
| MOTA | 15840 | CA | SER | 2353 | | | -27.085 | 75.051 | | 34.92 |
| MOTA | 15841 | CB | SER | 2353 | | | -27.483 | 75.815 | | 35.44 |
| MOTA | 15842 | OG | SER | 2353 | | | -26.429 | 76.657 | | 42.27 |
| MOTA | 15843 | С | SER | 2353 | | | -28.299 | 74.299 | | 34.42 |
| MOTA | 15844 | 0 | SER | 2353 | | | -29.186 | 74.889 | | 33.68 |
| MOTA | 15845 | N | GLY | 2354 | | 23.703 | -28.338 | 72.995 | 1.00 | 32.46 |
| ATOM | 15846 | CA | GLY | 2354 | | 24.150 | -29.463 | 72.198 | 1.00 | 31.21 |
| ATOM | 15847 | С | GLY | 2354 | | | -30.518 | 72.070 | 1.00 | 30.92 |
| ATOM | 15848 | 0 | GLY | 2354 | | 23.251 | -31.517 | 71.373 | 1.00 | 31.34 |
| ATOM | 15849 | N | VAL | 2355 | | 21.941 | -30.301 | 72.747 | 1.00 | 29.25 |
| MOTA | 15850 | CA | VAL | 2355 | | 20.814 | -31.235 | 72.702 | 1.00 | 29.20 |
| ATOM | 15851 | CB | VAL | 2355 | | 19.627 | -30.718 | 73.547 | 1.00 | 29.10 |
| ATOM | 15852 | CG1 | VAL | 2355 | | 18.484 | -31.725 | 73.510 | 1.00 | 29.45 |
| ATOM | 15853 | CG2 | VAL | 2355 | | 20.077 | -30.467 | 74.976 | 1.00 | 32.59 |
| ATOM | 15854 | С | VAL | 2355 | | 20.336 | -31.413 | 71.264 | 1.00 | 27.59 |
| MOTA | 15855 | 0 | VAL | 2355 | | 19.911 | -32.498 | 70.863 | 1.00 | 26.05 |
| ATOM | 15856 | N | TYR | 2356 | * | 20.399 | -30.330 | 70.498 | 1.00 | 28.08 |
| ATOM | 15857 | CA | TYR | 2356 | | 19.992 | -30.352 | 69.099 | 1.00 | 26.36 |
| ATOM | 15858 | CB | TYR | 2356 | | 18.713 | -29.543 | 68.889 | 1.00 | 25.86 |
| MOTA | 15859 | CG | TYR | 2356 | | 18.309 | -29.492 | 67.436 | 1.00 | 25.65 |
| ATOM | 15860 | CD1 | TYR | 2356 | | 17.733 | -30.602 | 66.817 | 1.00 | 25.65 |
| ATOM | 15861 | CE1 | TYR | 2356 | | 17.433 | -30.596 | 65.463 | 1.00 | 25.60 |
| ATOM | 15862 | CD2 | TYR | 2356 | | 18.569 | -28.363 | 66.659 | 1.00 | 24.57 |
| MOTA | 15863 | CE2 | TYR | 2356 | | | -28.345 | 65.299 | 1.00 | 24.48 |
| ATOM | 15864 | CZ | TYR | 2356 | | | -29.466 | 64.708 | | 25.02 |
| MOTA | 15865 | ОН | TYR | 2356 | | 17.423 | -29.471 | 63.361 | 1.00 | 25.86 |
| ATOM | 15866 | С | TYR | 2356 | | | -29.749 | 68.245 | | 27.03 |
| ATOM | 15867 | 0 | TYR | 2356 | | | -28.695 | 68.580 | | 26.04 |
| ATOM | 15868 | N | PRO | 2357 | | 21.437 | -30.405 | 67.124 | | 29.12 |
| ATOM | 15869 | CD | PRO | 2357 | | | -29.867 | 66.094 | | 29.21 |
| ATOM | 15870 | CA | PRO | 2357 | | | -31.650 | 66.668 | | 30.27 |
| ATOM | 15871 | CB | PRO | 2357 | | | -31.672 | 65.182 | 1.00 | 30.86 |
| ATOM | 15872 | CG | PRO | 2357 | | 22.494 | -31.034 | 65.145 | | 30.20 |
| ATOM | 15873 | C | PRO | 2357 | | | -32.886 | 67.397 | | 32.19 |
| MOTA | 15874 | ō | PRO | 2357. | | | -32.943 | 67.804 | | 31.74 |
| ATOM | 15875 | N | GLY | 2358 | | | -33.870 | 67.565 | | 33.64 |
| ATOM | 15876 | CA | GLY | 2358 | | | -35.094 | 68.236 | | 35.88 |
| ATOM | 15877 | C | GLY | 2358 | | | -36.113 | 67.222 | | 36.96 |
| MOTA | 15878 | | GLY | 2358 | | | -35.816 | 66.030 | | 34.73 |
| ATOM | 15879 | N | GLU | 2359 | | | -37.313 | 67.688 | | 38.39 |
| ATOM | 15880 | CA | GLU | 2359 | | | -38.369 | 66.795 | | 40.49 |
| ATOM | 15881 | CB | GLU | 2359 | | | -39.612 | 67.598 | | 42.44 |
| ATOM | 15882 | CG | GLU | 2359 | | | -40.830 | 66.733 | | 45.21 |
| ATOM | 15883 | CD | GLU | 2359 | | | -40.605 | 65.786 | | 46.88 |
| ATOM | 15884 | | GLU | 2359 | | | -41.352 | 64.786 | | 47.42 |
| ATOM | 15885 | | GLU | 2359 | | | -39.691 | 66.045 | | 48.14 |
| ATOM | 15886 | C | GLU | 2359 | | | -38.731 | 65.785 | | 41.07 |
| ATOM | 15887 | 0 | GLU | 2359 | | | -39.164 | 64.669 | | 40.53 |
| ATOM | 15888 | N | GLU | 2360 | | | -38.548 | 66.180 | | 40.84 |
| ATOM | 15889 | CA | GLU | 2360 | | | -38.862 | 65.302 | | 41.55 |
| ATOM | 15890 | CB | GLU | 2360 | | | -38.762 | 66.069 | | 43.54 |
| | | | | | | | | | | |

| ATOM | 15891 | CG | GLU | 2360 | 17.420 | -39.113 | 67.543 | 1.00 47.07 |
|---------|-------|-----|------|------|--------|---------|--------|------------|
| ATOM | 15892 | CD | GLU | 2360 | | -37.944 | 68.389 | 1.00 48.49 |
| | 15893 | OE1 | GLU | 2360 | 17.123 | -36.972 | 68.545 | 1.00 48.54 |
| MOTA | | | | 2360 | 19.040 | -37.993 | | 1.00 49.09 |
| MOTA | 15894 | OE2 | GLU | | | | 68.890 | |
| ATOM | 15895 | С | GLU | 2360 | 18.600 | -37.912 | 64.109 | 1.00 40.20 |
| MOTA | 15896 | 0 | GLU | 2360 | 18.018 | -38.231 | 63.073 | 1.00 40.08 |
| MOTA | 15897 | N | HIS | 2361 | 19.224 | -36.748 | 64.261 | 1.00 38.76 |
| MOTA | 15898 | CA | HIS | 2361 | 19.236 | -35.735 | 63.210 | 1.00 37.83 |
| ATOM | 15899 | CB | HIS | 2361 | 18.893 | -34.368 | 63.809 | 1.00 37.62 |
| ATOM | 15900 | CG | HIS | 2361 | 17.711 | -34.387 | 64.727 | 1.00 37.85 |
| ATOM | 15901 | CD2 | HIS | 2361 | 17.616 | -34.163 | 66.060 | 1.00 37.85 |
| ATOM | 15902 | | HIS | 2361 | 16.436 | -34.685 | 64.298 | 1.00 37.99 |
| ATOM | 15903 | | HIS | 2361 | 15.607 | -34.644 | 65.325 | 1.00 37.41 |
| ATOM | 15904 | | HIS | 2361 | 16.297 | -34.329 | 66.406 | 1.00 37.44 |
| ATOM | 15905 | C | HIS | 2361 | 20.588 | -35.639 | 62.514 | 1.00 37.16 |
| | 15905 | | | | | -34.739 | 61.704 | 1.00 37.10 |
| ATOM | | 0 | HIS | 2361 | | | | |
| MOTA | 15907 | N | SER | 2362 | | -36.569 | 62.829 | 1.00 37.15 |
| MOTA | 15908 | CA | SER | 2362 | | -36.561 | 62.251 | 1.00 37.47 |
| MOTA | 15909 | CB | SER | 2362 | 23.845 | -36.519 | 63.376 | 1.00 37.24 |
| MOTA | 15910 | OG | SER | 2362 | 23.557 | -35.456 | 64.274 | 1.00 38.09 |
| MOTA | 15911 | С | SER | 2362 | 23.087 | -37.757 | 61.342 | 1.00 38.18 |
| ATOM | 15912 | 0 | SER | 2362 | 22.511 | -38.831 | 61.519 | 1.00 37.89 |
| MOTA | 15913 | N | PHE | 2363 | 23.966 | -37.559 | 60.363 | 1.00 38.60 |
| ATOM | 15914 | CA | PHE | 2363 | 24.333 | -38.617 | 59.429 | 1.00 39.77 |
| ATOM | 15915 | CB | PHE | 2363 | 24.257 | -38.119 | 57.983 | 1.00 39.50 |
| ATOM | 15916 | CG. | PHE | 2363 | 22.932 | -37.524 | 57.613 | 1.00 39.62 |
| | | | | 2363 | 22.689 | -36.168 | 57.797 | 1.00 35.02 |
| ATOM | 15917 | | PHE | | | | | |
| ATOM | 15918 | | PHE | 2363 | 21.923 | -38.318 | 57.083 | 1.00 39.74 |
| ATOM | 15919 | | PHE | 2363 | 21.461 | -35.608 | 57.455 | 1.00 41.07 |
| ATOM | 15920 | CE2 | | 2363 | 20.690 | -37.769 | 56.737 | 1.00 40.32 |
| MOTA | 15921 | CZ | PHE | 2363 | 20.459 | -36.410 | 56.924 | 1.00 40.17 |
| MOTA | 15922 | С | PHE | 2363 | 25.756 | -39.089 | 59.719 | 1.00 40.49 |
| MOTA | 15923 | 0 | PHE | 2363 | 26.502 | -38.428 | 60.442 | 1.00 39.62 |
| ATOM | 15924 | N | HIS | 2364 | 26.129 | -40.228 | 59.145 | 1.00 41.96 |
| ATOM | 15925 | CA | HIS | 2364 | 27.462 | -40.791 | 59.336 | 1.00 44.57 |
| ATOM | 15926 | СВ | HIS | 2364 | 27.468 | -41.742 | 60.532 | 1.00 44.77 |
| ATOM | 15927 | CG | HIS | 2364 | 27.333 | -41.053 | 61.852 | 1.00 44.87 |
| | 15928 | | HIS | 2364 | 26.330 | -41.057 | 62.762 | 1.00 45.16 |
| MOTA | | | | | | | | |
| MOTA | 15929 | | HIS | 2364 | 28.310 | -40.227 | 62.363 | 1.00 45.32 |
| MOTA | 15930 | | HIS | 2364 | | -39.752 | 63.531 | 1.00 45.82 |
| MOTA | 15931 | | HIS | 2364 | | -40.241 | 63.796 | 1.00 45.37 |
| MOTA | 15932 | С | HIS | 2364 | 27.935 | -41.537 | 58.092 | 1.00 45.86 |
| MOTA | 15933 | 0 | HIS | 2364 | 29.117 | -41.375 | 57.723 | 1.00 47.15 |
| ATOM | 15934 | ОХТ | HIS | 2364 | 27.124 | -42.291 | 57.514 | 1.00 48.19 |
| ATOM | 15935 | C1 | KPL | 2365 | 18.263 | -24.454 | 54.329 | 1.00 39.29 |
| MOTA | 15936 | C2 | KPL. | 2365 | 19.445 | -23.498 | 54.099 | 1.00 40.45 |
| ATOM | 15937 | C3 | KPL | 2365 | 19.514 | -22.489 | 55.256 | 1.00 40.25 |
| MOTA | 15938 | C4 | KPL | 2365 | | -24.301 | 54.085 | 1.00 41.68 |
| ATOM | 15939 | 01 | KPL | 2365 | | -25.261 | 53.017 | 1.00 44.61 |
| ATOM | 15940 | C5 | KPL | 2365 | | -22.740 | 52.762 | 1.00 39.00 |
| | 15941 | 02 | | 2365 | 20.101 | -22.834 | 51.890 | 1.00 40.74 |
| MOTA | 15941 | C6 | | 2365 | | -21.873 | 52.491 | 1.00 40.74 |
| MOTA | | | | | | | | |
| MOTA | 15943 | 03 | KPL | 2365 | 17.180 | -21.735 | 53.324 | 1.00 37.05 |
| ATOM | 15944 | 04 | KPL | 2365 | 17.942 | -21.245 | 51.309 | 1.00 32.80 |
| MOTA | 15945 | CB | MET | 2401 | 40.796 | 32.161 | 43.908 | 1.00 71.21 |
| MOTA | 15946 | CG | MET | 2401 | 41.476 | 32.073 | 42.556 | 1.00 72.09 |
| MOTA | 15947 | SD | MET | 2401 | 42.294 | 33.600 | 42.104 | 1.00 73.69 |
| MOTA | 15948 | CE | MET | 2401 | 40.917 | 34.510 | 41.409 | 1.00 73.19 |
| ATOM | 15949 | С | MET | 2401 | 38.557 | 31.175 | 43.385 | 1.00 69.44 |
| ATOM | 15950 | 0 | MET | 2401 | 37.456 | 31.030 | 43.915 | 1.00 69.61 |
| ATOM | 15951 | N | MET | 2401 | 40.519 | 29.702 | 43.899 | 1.00 70.53 |
| ATOM | 15952 | CA | MET | 2401 | 39.842 | 30.999 | 44.194 | 1.00 70.42 |
| ATOM | 15953 | N | LYS | 2402 | 38.701 | 31.491 | 42.101 | 1.00 67.98 |
| MOTA | 15954 | CA | LYS | 2402 | 37.549 | 31.687 | 41.227 | 1.00 65.67 |
| | | | | | | 33.184 | 41.023 | 1.00 65.67 |
| ATOM | 15955 | CB | LYS | 2402 | 37.289 | | | |
| MOTA | 15956 | CG | LYS | 2402 | 36.953 | 33.945 | 42.298 | 1.00 67.98 |
| ATOM | 15957 | CD | LYS | 2402 | 35.541 | 33.652 | 42.783 | 1.00 68.89 |
| MOTA | 15958 | CE | LYS | 2402 | 34.501 | 34.222 | 41.830 | 1.00 69.72 |
| MOTA | 15959 | NZ | LYS | 2402 | 33.116 | 34.024 | 42.339 | 1.00 70.87 |
| MOTA | 15960 | С | LYS | 2402 | 37.781 | 31.021 | 39.875 | 1.00 62.73 |
| MOTA | 15961 | 0 | LYS | 2402 | 38.258 | 31.656 | 38.935 | 1.00 63.72 |
| ATOM | 15962 | N | PRO | 2403 | 37.454 | 29.725 | 39.763 | 1.00 59.41 |
| ATOM | 15963 | CD | PRO | 2403 | 37.320 | 29.060 | 38.454 | 1.00 58.79 |
| ATOM | 15964 | CA | PRO | 2403 | 36.895 | 28.884 | 40.825 | 1.00 55.82 |
| ATOM | 15965 | CB | PRO | 2403 | 35.981 | 27.948 | 40.054 | 1.00 57.33 |
| ATOM | 15966 | CG | PRO | 2403 | 36.797 | 27.681 | 38.829 | 1.00 58.38 |
| ATOM | 15967 | C | | | 37.987 | 28.122 | 41.576 | 1.00 52.24 |
| -11 011 | 10/01 | _ | PRO | 2403 | 31.301 | 20.122 | ==.0/0 | UU JA. 24 |

| ATOM | 15968 | 0 | PRO | 2403 | 39.149 | 28.127 | 41.170 | 1.00 51.69 |
|------|-------|-----|------|------|--------|--------|--------|------------|
| ATOM | 15969 | N | THR | 2404 | 37.605 | 27.465 | 42.667 | 1.00 47.66 |
| ATOM | 15970 | CA | THR | 2404 | 38.550 | 26.690 | 43.463 | 1.00 43.63 |
| | | | | 2404 | 37.971 | 26.341 | 44.846 | 1.00 43.73 |
| ATOM | 15971 | CB | THR | | | | | |
| ATOM | 15972 | OG1 | THR | 2404 | 37.739 | 27.544 | 45.588 | 1.00 43.30 |
| MOTA | 15973 | CG2 | THR | 2404 | 38.935 | 25.452 | 45.617 | 1.00 42.68 |
| ATOM | 15974 | C | THR | 2404 | 38.887 | 25.393 | 42.740 | 1.00 41.58 |
| MOTA | 15975 | 0 | THR | 2404 | 38.007 | 24.741 | 42.178 | 1.00 38.87 |
| MOTA | 15976 | N . | THR | 2405 | 40.163 | 25.022 | 42.762 | 1.00 40.92 |
| MOTA | 15977 | CA | THR | 2405 | 40.617 | 23.807 | 42.101 | 1.00 40.37 |
| ATOM | 15978 | CB | THR | 2405 | 41.289 | 24.127 | 40.753 | 1.00 40.36 |
| ATOM | 15979 | OG1 | THR | 2405 | 42.436 | 24.956 | 40.974 | 1.00 40.01 |
| ATOM | 15980 | CG2 | THR | 2405 | 40.317 | 24.849 | 39.832 | 1.00 39.63 |
| | | C | THR | 2405 | 41.607 | 23.020 | 42.954 | 1.00 40.56 |
| ATOM | 15981 | | | | | | | 1.00 39.81 |
| MOTA | 15982 | 0 | THR | 2405 | 42.106 | 23.514 | 43.966 | |
| MOTA | 15983 | N | ILE | 2406 | 41.883 | 21.790 | 42.531 | 1.00 40.97 |
| MOTA | 15984 | CA | ILE | 2406 | 42.815 | 20.909 | 43.228 | 1.00 41.27 |
| MOTA | 15985 | CB | ILE | 2406 | 43.064 | 19.621 | 42.414 | 1.00 41.43 |
| ATOM | 15986 | CG2 | ILE | 2406 | 43.817 | 18.602 | 43.264 | 1.00 39.98 |
| MOTA | 15987 | CG1 | ILE | 2406 | 41.730 | 19.036 | 41.949 | 1.00 42.65 |
| ATOM | 15988 | CD1 | ILE | 2406 | 41.859 | 18.074 | 40.783 | 1.00 44.77 |
| ATOM | 15989 | C | ILE | 2406 | 44.154 | 21.614 | 43.423 | 1.00 41.31 |
| ATOM | 15990 | ō | ILE | 2406 | 44.771 | 21.514 | 44.482 | 1.00 41.10 |
| ATOM | 15991 | N | SER | 2407 | 44.595 | 22.327 | 42.392 | 1.00 41.82 |
| | | | | | | | 42.442 | 1.00 42.16 |
| ATOM | 15992 | CA | SER | 2407 | 45.864 | 23.043 | | |
| ATOM | 15993 | CB | SER | 2407 | 46.042 | 23.881 | 41.175 | 1.00 42.77 |
| MOTA | 15994 | OG | SER | 2407 | 46.077 | 23.056 | 40.026 | 1.00 45.09 |
| MOTA | 15995 | C | SER | 2407 | 45.974 | 23.942 | 43.669 | 1.00 41.86 |
| MOTA | 15996 | 0 | SER | 2407 | 47.060 | 24.130 | 44.217 | 1.00 42.04 |
| MOTA | 15997 | N | LEU | 2408 | 44.846 | 24.495 | 44.101 | 1.00 41.20 |
| MOTA | 15998 | CA | LEU | 2408 | 44.838 | 25.374 | 45.262 | 1.00 40.42 |
| ATOM | 15999 | CB | LEU | 2408 | 43.483 | 26.071 | 45.390 | 1.00 41.71 |
| ATOM | 16000 | CG | LEU | 2408 | 43.521 | 27.558 | 45.753 | 1.00 42.81 |
| ATOM | 16001 | CD1 | | 2408 | 42.115 | 28.034 | 46.090 | 1.00 42.95 |
| | | | LEU | 2408 | 44.449 | 27.786 | 46.927 | 1.00 43.29 |
| ATOM | 16002 | | | | | | | 1.00 39.32 |
| ATOM | 16003 | С | LEU | 2408 | 45.126 | 24.580 | 46.533 | |
| MOTA | 16004 | 0 | LEU | 2408 | 45.921 | 25.004 | 47.372 | 1.00 38.69 |
| MOTA | 16005 | N | LEU | 2409 | 44.475 | 23.428 | 46.668 | 1.00 38.01 |
| MOTA | 16006 | CA | LEU | 2409 | 44.658 | 22.571 | 47.836 | 1.00 37.10 |
| MOTA | 16007 | CB | LEU | 2409 | 43.746 | 21.348 | 47.748 | 1.00 36.29 |
| MOTA | 16008 | CG | LEU | 2409 | 42.235 | 21.599 | 47.772 | 1.00 37.24 |
| ATOM | 16009 | CD1 | LEU | 2409 | 41.507 | 20.264 | 47.730 | 1.00 36.39 |
| ATOM | 16010 | CD2 | LEU | 2409 | 41.859 | 22.369 | 49.024 | 1.00 36.03 |
| ATOM | 16011 | C | LEU | 2409 | 46.103 | 22.113 | 47.956 | 1.00 37.48 |
| ATOM | 16012 | 0 | LEU | 2409 | 46.654 | 22.037 | 49.055 | 1.00 37.24 |
| ATOM | 16013 | N | GLN | 2410 | 46.711 | 21.805 | 46.815 | 1.00 37.94 |
| ATOM | 16014 | CA | GLN | 2410 | 48.096 | 21.356 | 46.779 | 1.00 38.43 |
| | 16014 | | GLN | 2410 | 48.487 | 20.989 | 45.346 | 1.00 38.65 |
| MOTA | | CB | | | | | 45.206 | 1.00 30.05 |
| ATOM | 16016 | CG | GLN | 2410 | 49.854 | 20.334 | | |
| ATOM | 16017 | CD | GLN | 2410 | 49.974 | 19.041 | 45.993 | 1.00 40.42 |
| ATOM | 16018 | | GLN | 2410 | 50.233 | 19.054 | 47.198 | 1.00 40.18 |
| MOTA | 16019 | NE2 | GLN | 2410 | 49.772 | 17.912 | 45.314 | 1.00 39.42 |
| MOTA | 16020 | С | GLN | 2410 | 48.986 | 22.477 | 47.299 | 1.00 38.19 |
| ATOM | 16021 | 0 | GLN | 2410 | 49.927 | 22.239 | 48.057 | 1.00 38.73 |
| ATOM | 16022 | N | LYS | 2411 | 48.676 | 23.701 | 46.888 | 1.00 38.25 |
| ATOM | 16023 | CA | LYS | 2411 | 49.431 | 24.866 | 47.324 | 1.00 38.59 |
| ATOM | 16024 | CB | LYS | 2411 | 48.887 | 26.129 | 46.652 | 1.00 40.48 |
| ATOM | 16025 | CG | LYS | 2411 | 49.561 | 27.410 | 47.114 | 1.00 44.48 |
| ATOM | 16026 | CD | LYS | 2411 | 48.792 | 28.639 | 46.664 | 1.00 46.76 |
| | 16027 | CE | | 2411 | 49.479 | 29.911 | 47.132 | 1.00 48.94 |
| MOTA | | | LYS | | | | | |
| ATOM | 16028 | NZ | LYS | 2411 | 48.656 | 31.123 | 46.857 | 1.00 51.10 |
| MOTA | 16029 | С | LYS | 2411 | 49.313 | 25.009 | 48.839 | 1.00 37.82 |
| MOTA | 16030 | 0 | LYS | 2411 | 50.300 | 25.261 | 49.533 | 1.00 36.98 |
| MOTA | 16031 | N | TYR | 2412 | 48.094 | 24.846 | 49.346 | 1.00 36.70 |
| MOTA | 16032 | CA | TYR | 2412 | 47.839 | 24.959 | 50.776 | 1.00 36.04 |
| MOTA | 16033 | CB | TYR- | 2412 | 46.364 | 24.667 | 51.075 | 1.00 38.21 |
| MOTA | 16034 | CG | TYR | 2412 | 45.409 | 25.792 | 50.731 | 1.00 39.60 |
| ATOM | 16035 | CD1 | TYR | 2412 | 44.029 | 25.579 | 50.728 | 1.00 41.45 |
| ATOM | 16036 | CE1 | TYR | 2412 | 43.137 | 26.615 | 50.450 | 1.00 42.37 |
| ATOM | 16037 | CD2 | TYR | 2412 | 45.877 | 27.075 | 50.444 | 1.00 40.64 |
| ATOM | 16038 | CE2 | | 2412 | 44.995 | 28.117 | 50.166 | 1.00 41.94 |
| ATOM | 16039 | CZ | TYR | 2412 | 43.626 | 27.879 | 50.172 | 1.00 42.98 |
| | | | | 2412 | 42.746 | 28.905 | 49.908 | 1.00 45.55 |
| ATOM | 16040 | ОН | TYR | | | | | |
| ATOM | 16041 | С | TYR | 2412 | 48.726 | 24.020 | 51.587 | 1.00 33.83 |
| ATOM | 16042 | 0 | TYR | 2412 | 49.264 | 24.408 | 52.621 | 1.00 32.94 |
| MOTA | 16043 | N | LYS | 2413 | 48.884 | 22.787 | 51.118 | 1.00 32.53 |
| MOTA | 16044 | CA | LYS | 2413 | 49.711 | 21.825 | 51.832 | 1.00 34.20 |
| | | | | | | | | |

| ATOM | 16045 | СВ | LYS | 2413 | 49.613 | 20.437 | 51.197 | 1.00 32.95 |
|------|-------|-----|-----|------|--------|--------|--------|------------|
| ATOM | 16046 | CG | LYS | 2413 | 50.515 | 19.412 | 51.871 | 1.00 31.62 |
| ATOM | 16047 | CD | LYS | 2413 | 50.181 | 17.995 | 51.455 | 1.00 30.68 |
| | | | | | | | 52.235 | 1.00 29.20 |
| ATOM | 16048 | CE | LYS | 2413 | 51.017 | 16.996 | | |
| ATOM | 16049 | NZ | LYS | 2413 | 50.512 | 15.606 | 52.122 | 1.00 28.10 |
| MOTA | 16050 | С | LYS | 2413 | 51.168 | 22.266 | 51.848 | 1.00 34.97 |
| ATOM | 16051 | 0 | LYS | 2413 | 51.864 | 22.101 | 52.848 | 1.00 33.55 |
| ATOM | 16052 | N | GLN | 2414 | 51.629 | 22.815 | 50.730 | 1.00 37.13 |
| ATOM | 16053 | CA | GLN | 2414 | 53.002 | 23.282 | 50.631 | 1.00 40.24 |
| ATOM | 16054 | СВ | GLN | 2414 | 53.301 | 23.745 | 49.207 | 1.00 43.05 |
| ATOM | 16055 | CG | GLN | 2414 | 53.429 | 22.605 | 48.210 | 1.00 47.04 |
| | | | | | 53.593 | | 46.784 | 1.00 47.04 |
| ATOM | 16056 | CD | GLN | 2414 | | 23.099 | | |
| ATOM | 16057 | OE1 | | 2414 | 54.346 | 24.043 | 46.523 | 1.00 51.23 |
| MOTA | 16058 | NE2 | GLN | 2414 | 52.897 | 22.457 | 45.850 | 1.00 49.77 |
| MOTA | 16059 | С | GLN | 2414 | 53.228 | 24.425 | 51.609 | 1.00 41.12 |
| MOTA | 16060 | 0 | GLN | 2414 | 54.266 | 24.494 | 52.267 | 1.00 41.34 |
| ATOM | 16061 | N | GLU | 2415 | 52.247 | 25.315 | 51.704 | 1.00 41.66 |
| ATOM | 16062 | CA | GLU | 2415 | 52.325 | 26.454 | 52.609 | 1.00 42.25 |
| ATOM | 16063 | CB | GLU | 2415 | 51.333 | 27.536 | 52.180 | 1.00 43.79 |
| ATOM | 16064 | CG | GLU | 2415 | 51.495 | 27.981 | 50.740 | 1.00 46.53 |
| ATOM | 16065 | CD | GLU | 2415 | 50.637 | 29.182 | 50.404 | 1.00 47.48 |
| | | | | | | | 50.564 | 1.00 47.48 |
| ATOM | 16066 | OE1 | GLU | 2415 | 49.401 | 29.100 | | |
| ATOM | 16067 | OE2 | GLU | 2415 | 51.202 | 30.212 | 49.979 | 1.00 49.09 |
| MOTA | 16068 | С | GLU | 2415 | 52.011 | 26.010 | 54.034 | 1.00 41.63 |
| ATOM | 16069 | 0 | GLU | 2415 | 52.000 | 26.820 | 54.964 | 1.00 41.75 |
| ATOM | 16070 | N | LYS | 2416 | 51.753 | 24.716 | 54.194 | 1.00 40.45 |
| ATOM | 16071 | CA | LYS | 2416 | 51.435 | 24.143 | 55.496 | 1.00 40.01 |
| ATOM | 16072 | CB | LYS | 2416 | 52.607 | 24.345 | 56.458 | 1.00 42.70 |
| ATOM | 16073 | CG | LYS | 2416 | 53.969 | 24.092 | 55.830 | 1.00 45.22 |
| ATOM | 16074 | CD | LYS | 2416 | 54.093 | 22.669 | 55.316 | 1.00 47.92 |
| | | CE | LYS | 2416 | 55.361 | 22.490 | 54.492 | 1.00 49.09 |
| ATOM | 16075 | | | | | | | |
| ATOM | 16076 | NZ | LYS | 2416 | 56.586 | 22.872 | 55.248 | 1.00 50.44 |
| MOTA | 16077 | С | LYS | 2416 | 50.177 | 24.784 | 56.077 | 1.00 38.54 |
| MOTA | 16078 | 0 | LYS | 2416 | 50.012 | 24.850 | 57.295 | 1.00 38.60 |
| MOTA | 16079 | N | LYS | 2417 | 49.296 | 25.266 | 55.205 | 1.00 36.93 |
| MOTA | 16080 | CA | LYS | 2417 | 48.053 | 25.891 | 55.644 | 1.00 34.59 |
| MOTA | 16081 | CB | LYS | 2417 | 47.682 | 27.061 | 54.727 | 1.00 35.93 |
| ATOM | 16082 | CG | LYS | 2417 | 46.420 | 27.802 | 55.159 | 1.00 36.62 |
| ATOM | 16083 | CD | LYS | 2417 | 45.948 | 28.803 | 54.106 | 1.00 40.30 |
| ATOM | 16084 | CE | LYS | 2417 | 46.952 | 29.928 | 53.890 | 1.00 41.87 |
| | | | | | | | | |
| ATOM | 16085 | NZ | LYS | 2417 | 46.553 | 30.824 | 52.762 | 1.00 42.71 |
| MOTA | 16086 | С | LYS | 2417 | 46.917 | 24.873 | 55.641 | 1.00 33.02 |
| ATOM | 16087 | 0 | LYS | 2417 | 46.510 | 24.388 | 54.584 | 1.00 31.46 |
| MOTA | 16088 | N | ARG | 2418 | 46.414 | 24.552 | 56.829 | 1.00 31.31 |
| MOTA | 16089 | CA | ARG | 2418 | 45.320 | 23.595 | 56.968 | 1.00 29.79 |
| MOTA | 16090 | CB | ARG | 2418 | 45.198 | 23.161 | 58.429 | 1.00 30.22 |
| ATOM | 16091 | CG | ARG | 2418 | 46.304 | 22.203 | 58.847 | 1.00 31.76 |
| ATOM | 16092 | CD | ARG | 2418 | 46.446 | 22.096 | 60.355 | 1.00 33.22 |
| ATOM | 16093 | NE | ARG | 2418 | 46.949 | 23.344 | 60.925 | 1.00 34.67 |
| ATOM | 16094 | CZ | ARG | 2418 | 47.516 | 23.446 | 62.122 | 1.00 34.59 |
| | 16095 | | | | 47.659 | 22.371 | | 1.00 35.64 |
| ATOM | | | ARG | 2418 | | | 62.884 | |
| ATOM | 16096 | | ARG | | | 24.623 | | |
| MOTA | 16097 | C | ARG | 2418 | 44.011 | 24.195 | 56.466 | 1.00 28.42 |
| MOTA | 16098 | 0 | ARG | 2418 | 43.638 | 25.300 | 56.854 | 1.00 28.67 |
| MOTA | 16099 | N | PHE | 2419 | 43.318 | 23.454 | 55.603 | 1.00 27.53 |
| MOTA | 16100 | CA | PHE | 2419 | 42.065 | 23.915 | 55.005 | 1.00 24.08 |
| ATOM | 16101 | CB | PHE | 2419 | 42.198 | 23.883 | 53.478 | 1.00 25.14 |
| ATOM | 16102 | CG | PHE | 2419 | 42.502 | 22.519 | 52.917 | 1.00 27.81 |
| ATOM | 16103 | | PHE | 2419 | 41.472 | 21.650 | 52.560 | 1.00 27.73 |
| ATOM | 16104 | | PHE | 2419 | 43.821 | 22.100 | 52.742 | 1.00 27.96 |
| ATOM | 16105 | | PHE | 2419 | 41.748 | 20.387 | 52.036 | 1.00 26.05 |
| ATOM | 16105 | | PHE | 2419 | 44.109 | 20.836 | 52.218 | 1.00 28.62 |
| | | | | | | | | 1.00 28.62 |
| ATOM | 16107 | CZ | PHE | 2419 | 43.070 | 19.978 | 51.864 | |
| ATOM | 16108 | С | PHE | 2419 | 40.837 | 23.110 | 55.439 | 1.00 22.88 |
| ATOM | 16109 | 0 | PHE | 2419 | 40.930 | 21.924 | 55.734 | 1.00 19.16 |
| MOTA | 16110 | N | ALA | 2420 | 39.684 | 23.768 | 55.476 | 1.00 21.94 |
| MOTA | 16111 | CA | ALA | 2420 | 38.456 | 23.100 | 55.872 | 1.00 22.77 |
| ATOM | 16112 | CB | ALA | 2420 | 37.617 | 24.027 | 56.757 | 1.00 21.44 |
| ATOM | 16113 | С | ALA | 2420 | 37.640 | 22.656 | 54.660 | 1.00 22.17 |
| MOTA | 16114 | 0 | ALA | 2420 | 37.611 | 23.332 | 53.626 | 1.00 22.74 |
| MOTA | 16115 | N | THR | 2421 | 36.977 | 21.512 | 54.802 | 1.00 22.82 |
| ATOM | 16116 | CA | THR | 2421 | 36.138 | 20.942 | 53.750 | 1.00 22.02 |
| ATOM | 16117 | CB | THR | 2421 | 36.814 | 19.711 | 53.730 | 1.00 24.06 |
| MOTA | | OG1 | | | 38.061 | | | 1.00 24.00 |
| | 16118 | | THR | 2421 | | 20.108 | 52.514 | |
| MOTA | 16119 | CG2 | THR | 2421 | 35.923 | 19.109 | 52.048 | 1.00 27.64 |
| ATOM | 16120 | С | THR | 2421 | 34.839 | 20.509 | 54.419 | 1.00 18.96 |
| MOTA | 16121 | 0 | THR | 2421 | 34.814 | 20.246 | 55.619 | 1.00 18.47 |
| | | | | | | | | |

| ATOM | 16122 | N | ILE | 2422 | 33.759 | 20.422 | 53.656 | 1.00 19.02 |
|------|-------|-----------|------|------|--------|--------|--------|------------|
| ATOM | 16123 | CA | ILE | 2422 | 32.487 | 20.040 | 54.257 | 1.00 17.25 |
| MOTA | 16124 | CB | ILE | 2422 | 31.764 | 21.296 | 54.811 | 1.00 19.41 |
| ATOM | 16125 | CG2 | ILE | 2422 | 31.183 | 22.112 | 53.667 | 1.00 20.48 |
| ATOM | 16126 | CG1 | ILE | 2422 | 30.664 | 20.889 | 55.792 | 1.00 21.17 |
| MOTA | 16127 | CD1 | ILE | 2422 | 30.129 | 22.046 | 56.604 | 1.00 25.73 |
| ATOM | 16128 | C | ILE | 2422 | 31.574 | 19.332 | 53.269 | 1.00 17.99 |
| ATOM | 16129 | 0 | ILE | 2422 | 31.726 | 19.474 | 52.059 | 1.00 16.35 |
| | 16130 | N | THR | 2423 | 30.625 | 18.569 | 53.793 | 1.00 17.55 |
| ATOM | | | | 2423 | 29.686 | 17.873 | 52.932 | 1.00 17.33 |
| ATOM | 16131 | CA | THR | | | | | |
| ATOM | 16132 | CB | THR | 2423 | 29.163 | 16.577 | 53.580 | 1.00 21.53 |
| ATOM | 16133 | OG1 | THR | 2423 | 28.287 | 16.899 | 54.668 | 1.00 22.21 |
| ATOM | 16134 | CG2 | THR | 2423 | 30.327 | 15.738 | 54.098 | 1.00 26.19 |
| ATOM | 16135 | С | THR | 2423 | 28.514 | 18.815 | 52.682 | 1.00 19.08 |
| ATOM | 16136 | 0 | THR | 2423 | 28.210 | 19.678 | 53.504 | 1.00 18.44 |
| MOTA | 16137 | N | ALA | 2424 | 27.877 | 18.661 | 51.527 | 1.00 18.78 |
| MOTA | 16138 | CA | ALA | 2424 | 26.730 | 19.476 | 51.154 | 1.00 16.80 |
| MOTA | 16139 | CB | ALA | 2424 | 27.180 | 20.720 | 50.394 | 1.00 17.89 |
| ATOM | 16140 | С | ALA. | 2424 | 25.843 | 18.614 | 50.269 | 1.00 17.29 |
| MOTA | 16141 | 0 | ALA | 2424 | 26.342 | 17.787 | 49.510 | 1.00 15.04 |
| MOTA | 16142 | N | TYR | 2425 | 24.532 | 18.795 | 50.361 | 1.00 16.73 |
| MOTA | 16143 | CA | TYR | 2425 | 23.633 | 17.982 | 49.547 | 1.00 17.37 |
| ATOM | 16144 | CB | TYR | 2425 | 23.040 | 16.852 | 50.387 | 1.00 16.33 |
| ATOM | 16145 | CG | TYR | 2425 | 24.006 | 16.220 | 51.351 | 1.00 17.54 |
| ATOM | 16146 | CD1 | TYR | 2425 | 23.974 | 16.546 | 52.704 | 1.00 18.85 |
| ATOM | 16147 | CE1 | TYR | 2425 | 24.846 | 15.954 | 53.605 | 1.00 19.50 |
| ATOM | 16148 | CD2 | | 2425 | 24.946 | 15.285 | 50.917 | 1.00 17.67 |
| ATOM | 16149 | | TYR | 2425 | 25.829 | 14.684 | 51.815 | 1.00 18.16 |
| ATOM | 16150 | CZ | TYR | 2425 | 25.766 | 15.026 | 53.160 | 1.00 19.76 |
| ATOM | 16151 | OH | TYR | 2425 | 26.608 | 14.418 | 54.065 | 1.00 21.42 |
| ATOM | 16152 | C | TYR | 2425 | 22.496 | 18.760 | 48.908 | 1.00 18.27 |
| ATOM | 16153 | o | TYR | 2425 | 21.639 | 18.172 | 48.248 | 1.00 20.53 |
| ATOM | 16154 | N | ASP | 2426 | 22.477 | 20.074 | 49.101 | 1.00 17.43 |
| ATOM | 16155 | CA | ASP | 2426 | 21.420 | 20.899 | 48.525 | 1.00 17.57 |
| ATOM | 16156 | CB | ASP | 2426 | 20.228 | 20.964 | 49.486 | 1.00 17.38 |
| | | | | 2426 | 20.581 | 21.617 | 50.824 | 1.00 17.35 |
| MOTA | 16157 | CG OD1 | ASP | | | | 50.824 | 1.00 20.93 |
| ATOM | 16158 | OD1 | | 2426 | 20.752 | 22.849 | | |
| ATOM | 16159 | OD2 | | 2426 | 20.687 | 20.892 | 51.836 | 1.00 19.12 |
| ATOM | 16160 | C | ASP | 2426 | 21.904 | 22.309 | 48.195 | 1.00 19.13 |
| ATOM | 16161 | 0 | ASP | 2426 | 22.985 | 22.720 | 48.615 | 1.00 19.45 |
| ATOM | 16162 | N | TYR | 2427 | 21.084 | 23.040 | 47.448 | 1.00 17.80 |
| MOTA | 16163 | CA | TYR | 2427 | 21.385 | 24.404 | 47.026 | 1.00 20.14 |
| MOTA | 16164 | CB | TYR | 2427 | 20.232 | 24.941 | 46.175 | 1.00 19.94 |
| MOTA | 16165 | CG | TYR | 2427 | 20.321 | 26.420 | 45.862 | 1.00 20.70 |
| MOTA | 16166 | | TYR | 2427 | 21.142 | 26.891 | 44.838 | 1.00 20.50 |
| MOTA | 16167 | | TYR | 2427 | 21.222 | 28.253 | 44.547 | 1.00 23.68 |
| MOTA | 16168 | CD2 | TYR | 2427 | 19.581 | 27.351 | 46.594 | 1.00 23.01 |
| MOTA | 16169 | CE2 | TYR | 2427 | 19.652 | 28.711 | 46.314 | 1.00 23.40 |
| MOTA | 16170 | CZ | TYR | 2427 | 20.470 | 29.156 | 45.291 | 1.00 24.74 |
| MOTA | 16171 | ОН | TYR | 2427 | 20.526 | 30.499 | 45.006 | 1.00 28.18 |
| MOTA | 16172 | С | TYR | 2427 | 21.630 | 25.382 | 48.174 | 1.00 20.13 |
| ATOM | 16173 | 0 | TYR | 2427 | 22.609 | 26.124 | 48.163 | 1.00 19.70 |
| MOTA | 16174 | N | SER | 2428 | 20.727 | 25.379 | 49.148 | 1.00 20.69 |
| MOTA | 16175 | CA | SER | 2428 | 20.794 | 26.288 | 50.287 | 1.00 20.45 |
| MOTA | 16176 | CB | SER | 2428 | 19.592 | 26.055 | 51.200 | 1.00 21.08 |
| MOTA | 16177 | OG | SER | 2428 | 18.394 | 26.357 | 50.511 | 1.00 19.23 |
| MOTA | 16178 | С | SER | 2428 | 22.077 | 26.252 | 51.107 | 1.00 20.33 |
| ATOM | 16179 | 0 | SER | 2428 | 22.717 | 27.289 | 51.328 | 1.00 19.96 |
| ATOM | 16180 | N | PHE | 2429 | 22.456 | 25.073 | 51.580 | 1.00 18.92 |
| ATOM | 16181 | CA | PHE | 2429 | 23.678 | 24.976 | 52.363 | 1.00 18.46 |
| ATOM | 16182 | CB | PHE | 2429 | 23.739 | 23.643 | 53.120 | 1.00 17.47 |
| ATOM | 16183 | CG | PHE | 2429 | 22.916 | 23.633 | 54.381 | 1.00 18.24 |
| ATOM | 16184 | | PHE | 2429 | 21.682 | 22.986 | 54.427 | 1.00 17.48 |
| MOTA | 16185 | | PHE | 2429 | 23.370 | 24.296 | 55.524 | 1.00 15.99 |
| ATOM | 16186 | | PHE | 2429 | 20.911 | 22.995 | 55.590 | 1.00 17.58 |
| MOTA | 16187 | | PHE | 2429 | 22.611 | 24.312 | 56.686 | 1.00 13.97 |
| ATOM | 16188 | CZ | PHE | 2429 | 21.376 | 23.661 | 56.727 | 1.00 17.59 |
| ATOM | 16189 | C | PHE | 2429 | 24.917 | 25.174 | 51.496 | 1.00 17.35 |
| ATOM | 16190 | 0 | PHE | 2429 | 25.885 | 25.813 | 51.924 | 1.00 19.44 |
| | | | | | 24.892 | 24.653 | 50.271 | 1.00 18.28 |
| MOTA | 16191 | N | ALA | 2430 | 26.035 | 24.653 | 49.381 | 1.00 20.34 |
| ATOM | 16192 | CA | ALA | 2430 | | | 48.064 | 1.00 22.75 |
| ATOM | 16193 | CB | ALA | 2430 | 25.805 | 24.092 | | |
| MOTA | 16194 | С | ALA | 2430 | 26.251 | 26.325 | 49.119 | 1.00 23.92 |
| ATOM | 16195 | 0 | ALA | 2430 | 27.388 | 26.792 | 49.003 | 1.00 25.09 |
| MOTA | 16196 | N | LYS | 2431 | 25.148 | 27.065 | 49.037 | 1.00 24.33 |
| ATOM | 16197 | CA | LYS | 2431 | 25.180 | 28.506 | 48.797 | 1.00 25.15 |
| ATOM | 16198 | CB | LYS | 2431 | 23.767 | 28.999 | 48.460 | 1.00 27.16 |
| | | | | | | | | |

| ATOM | 16199 | CG | LYS | 2431 | 23.646 | 30.478 | 48.124 | 1.00 29.73 |
|------|-------|-----|-----|------|--------|--------|--------|------------|
| ATOM | 16200 | CD | LYS | 2431 | 24.318 | 30.816 | 46.811 | 1.00 34.33 |
| ATOM | 16201 | CE | LYS | 2431 | 23.775 | 32.117 | 46.241 | 1.00 37.47 |
| MOTA | 16202 | NZ | LYS | 2431 | 23.956 | 33.264 | 47.174 | 1.00 39.95 |
| ATOM | 16203 | C | LYS | 2431 | 25.712 | 29.246 | 50.027 | 1.00 24.27 |
| ATOM | 16204 | 0 | LYS | 2431 | 26.546 | 30.145 | 49.918 | 1.00 23.43 |
| ATOM | 16205 | N | LEU | 2432 | 25.219 | 28.858 | 51.198 | 1.00 23.70 |
| ATOM | 16206 | CA | LEU | 2432 | 25.641 | 29.468 | 52.451 | 1.00 23.86 |
| ATOM | 16207 | CB | LEU | 2432 | 24.812 | 28.898 | 53.609 | 1.00 21.16 |
| ATOM | 16208 | CG | LEU | 2432 | 25.055 | 29.415 | 55.035 | 1.00 19.80 |
| ATOM | 16209 | CD1 | LEU | 2432 | 23.849 | 29.079 | 55.909 | 1.00 16.46 |
| ATOM | 16210 | | LEU | 2432 | 26.322 | 28.796 | 55.613 | 1.00 16.28 |
| MOTA | 16211 | C | LEU | 2432 | 27.132 | 29.240 | 52.697 | 1.00 24.74 |
| MOTA | 16212 | 0 | LEU | 2432 | 27.825 | 30.134 | 53.180 | 1.00 25.72 |
| ATOM | 16213 | N | PHE | 2433 | 27.630 | 28.051 | 52.367 | 1.00 25.69 |
| ATOM | 16214 | CA | PHE | 2433 | 29.049 | 27.752 | 52.567 | 1.00 25.88 |
| ATOM | 16215 | CB | PHE | 2433 | 29.343 | 26.259 | 52.358 | 1.00 25.66 |
| MOTA | 16216 | CG | PHE | 2433 | 28.615 | 25.342 | 53.307 | 1.00 23.12 |
| ATOM | 16217 | CD1 | PHE | 2433 | 28.351 | 25.728 | 54.621 | 1.00 20.93 |
| ATOM | 16218 | CD2 | PHE | 2433 | 28.204 | 24.076 | 52.884 | 1.00 22.54 |
| ATOM | 16219 | CE1 | PHE | 2433 | 27.688 | 24.873 | 55.499 | 1.00 21.36 |
| ATOM | 16220 | CE2 | PHE | 2433 | 27.542 | 23.214 | 53.756 | 1.00 21.24 |
| ATOM | 16221 | CZ | PHE | 2433 | 27.281 | 23.613 | 55.068 | 1.00 23.36 |
| ATOM | 16222 | С | PHE | 2433 | 29.918 | 28.557 | 51.606 | 1.00 28.10 |
| ATOM | 16223 | 0 | PHE | 2433 | 30.890 | 29.192 | 52.019 | 1.00 26.80 |
| ATOM | 16224 | N | ALA | 2434 | 29.575 | 28.520 | 50.319 | 1.00 28.19 |
| MOTA | 16225 | CA | ALA | 2434 | 30.341 | 29.250 | 49.314 | 1.00 29.37 |
| MOTA | 16226 | CB | ALA | 2434 | 29.714 | 29.072 | 47.934 | 1.00 28.66 |
| ATOM | 16227 | С | ALA | 2434 | 30.424 | 30.731 | 49.665 | 1.00 29.43 |
| ATOM | 16228 | 0 | ALA | 2434 | 31.465 | 31.358 | 49.480 | 1.00 29.86 |
| ATOM | 16229 | N | ASP | 2435 | 29.331 | 31.289 | 50.176 | 1.00 29.97 |
| ATOM | 16230 | CA | ASP | 2435 | 29.320 | 32.702 | 50.540 | 1.00 32.22 |
| ATOM | 16231 | CB | ASP | 2435 | 27.893 | 33.205 | 50.766 | 1.00 33.58 |
| MOTA | 16232 | CG | ASP | 2435 | 27.021 | 33.062 | 49.539 | 1.00 36.19 |
| ATOM | 16233 | OD1 | ASP | 2435 | 27.540 | 33.202 | 48.409 | 1.00 37.94 |
| ATOM | 16234 | OD2 | ASP | 2435 | 25.807 | 32.825 | 49.706 | 1.00 38.98 |
| ATOM | 16235 | С | ASP | 2435 | 30.143 | 32.997 | 51.787 | 1.00 32.06 |
| ATOM | 16236 | 0 | ASP | 2435 | 30.372 | 34.161 | 52.117 | 1.00 32.90 |
| ATOM | 16237 | N | GLU | 2436 | 30.580 | 31.955 | 52.486 | 1.00 31.24 |
| ATOM | 16238 | CA | GLU | 2436 | 31.376 | 32.149 | 53.687 | 1.00 31.97 |
| ATOM | 16239 | CB | GLU | 2436 | 30.816 | 31.326 | 54.850 | 1.00 32.11 |
| ATOM | 16240 | CG | GLU | 2436 | 29.464 | 31.801 | 55.357 | 1.00 33.39 |
| ATOM | 16241 | CD | GLU | 2436 | 29.453 | 33.285 | 55.680 | 1.00 33.83 |
| ATOM | 16242 | OE1 | GLU | 2436 | 30.357 | 33.745 | 56.411 | 1.00 35.70 |
| ATOM | 16243 | OE2 | GLU | 2436 | 28.537 | 33.987 | 55.208 | 1.00 33.76 |
| ATOM | 16244 | C | GLU | 2436 | 32.836 | 31.790 | 53.472 | 1.00 32.46 |
| ATOM | 16245 | 0 | GLU | 2436 | 33.659 | 31.983 | 54.362 | 1.00 32.04 |
| ATOM | 16246 | N | GLY | 2437 | 33.162 | 31.265 | 52.294 | 1.00 32.25 |
| ATOM | 16247 | CA | GLY | 2437 | 34.542 | 30.904 | 52.026 | 1.00 33.78 |
| ATOM | 16248 | C | GLY | 2437 | 34.786 | 29.425 | 51.797 | 1.00 33.68 |
| ATOM | 16249 | 0 | GLY | 2437 | 35.759 | 29.062 | 51.143 | 1.00 36.34 |
| ATOM | 16250 | N | LEU | 2438 | 33.927 | 28.569 | 52.347 | 1.00 32.66 |
| MOTA | 16251 | CA | LEU | 2438 | 34.066 | 27.127 | 52.161 | 1.00 32.08 |
| MOTA | 16252 | CB | LEU | 2438 | 33.059 | 26.372 | 53.031 | 1.00 32.00 |
| MOTA | 16253 | CG | LEU | 2438 | 33.606 | 25.758 | 54.314 | 1.00 31.91 |
| MOTA | 16254 | CD1 | LEU | 2438 | 32.472 | 25.144 | 55.116 | 1.00 31.31 |
| MOTA | 16255 | CD2 | LEU | 2438 | 34.656 | 24.708 | 53.977 | 1.00 32.09 |
| ATOM | 16256 | С | LEU | 2438 | 33.810 | 26.810 | 50.697 | 1.00 30.44 |
| ATOM | 16257 | 0 | LEU | 2438 | 32.659 | 26.721 | 50.267 | 1.00 30.98 |
| MOTA | 16258 | N | ASN | 2439 | 34.889 | 26.641 | 49.940 | 1.00 29.40 |
| MOTA | 16259 | CA | ASN | 2439 | 34.788 | 26.370 | 48.513 | 1.00 28.49 |
| ATOM | 16260 | CB | ASN | 2439 | 35.721 | 27.306 | 47.738 | 1.00 31.32 |
| MOTA | 16261 | CG | ASN | 2439 | 35.549 | 28.764 | 48.134 | 1.00 34.03 |
| ATOM | 16262 | OD1 | ASN | 2439 | 34.435 | 29.292 | 48.140 | 1.00 36.11 |
| ATOM | 16263 | ND2 | ASN | 2439 | 36.655 | 29.422 | 48.461 | 1.00 35.10 |
| ATOM | 16264 | С | ASN | 2439 | 35.122 | 24.922 | 48.173 | 1.00 26.24 |
| MOTA | 16265 | 0 | ASN | | 35.344 | | | 1.00 25.25 |
| MOTA | 16266 | N | VAL | 2440 | 35.155 | 24.065 | 49.188 | 1.00 24.29 |
| MOTA | 16267 | CA | VAL | 2440 | 35.446 | 22.657 | 48.985 | 1.00 24.09 |
| MOTA | 16268 | CB | VAL | 2440 | 36.774 | 22.248 | 49.640 | 1.00 25.05 |
| MOTA | 16269 | | VAL | 2440 | 37.067 | 20.788 | 49.345 | 1.00 24.91 |
| MOTA | 16270 | | VAL | 2440 | 37.896 | 23.126 | 49.114 | 1.00 25.37 |
| ATOM | 16271 | C | VAL | 2440 | 34.323 | 21.843 | 49.597 | 1.00 22.62 |
| ATOM | 16272 | 0 | VAL | 2440 | 34.228 | 21.711 | 50.816 | 1.00 19.04 |
| ATOM | 16273 | N | MET | 2441 | 33.471 | 21.297 | 48.737 | 1.00 21.81 |
| MOTA | 16274 | CA | MET | 2441 | 32.322 | 20.528 | 49.183 | 1.00 20.07 |
| MOTA | 16275 | CB | MET | 2441 | 31.033 | 21.250 | 48.785 | 1.00 22.11 |
| | | | | | | | | |

| ATOM | 16276 | CG | MET | 2441 | | 30.682 | 22.414 | 49.695 | 1.00 | 23.98 |
|------|-------|------|-----|------|---|--------|--------|--------|------|-------|
| ATOM | 16277 | SD | MET | 2441 | | 29.512 | 23.563 | 48.974 | | 25.48 |
| ATOM | 16278 | CE | MET | 2441 | | 30.566 | 25.021 | 48.739 | | 24.85 |
| ATOM | 16279 | c | MET | 2441 | | 32.295 | 19.118 | 48.637 | | 20.47 |
| ATOM | 16280 | ŏ | MET | 2441 | | 32.712 | 18.867 | 47.508 | | 19.61 |
| ATOM | 16281 | N | LEU | 2442 | | 31.786 | 18.200 | 49.450 | | 19.57 |
| ATOM | 16282 | CA | LEU | 2442 | | 31.689 | 16.805 | 49.055 | | 20.14 |
| ATOM | 16283 | СВ | LEU | 2442 | | 32.576 | 15.951 | 49.964 | | 20.82 |
| ATOM | 16284 | CG | LEU | 2442 | | 32.654 | 14.421 | 49.855 | | 24.63 |
| ATOM | 16285 | CD1 | | 2442 | | 31.547 | 13.810 | 50.661 | | 25.41 |
| ATOM | 16286 | CD2 | | 2442 | | 32.611 | 13.956 | 48.399 | | 22.10 |
| ATOM | 16287 | C | LEU | 2442 | | 30.254 | 16.307 | 49.104 | | 18.06 |
| ATOM | 16288 | ō | LEU | 2442 | | 29.556 | 16.453 | 50.109 | | 15.33 |
| ATOM | 16289 | N | VAL | 2443 | | 29.816 | 15.730 | 47.998 | | 16.74 |
| ATOM | 16290 | CA | VAL | 2443 | • | 28.481 | 15.155 | 47.931 | | 18.13 |
| ATOM | 16291 | CB | VAL | 2443 | | 27.850 | 15.367 | 46.553 | | 18.92 |
| ATOM | 16292 | CG1 | VAL | 2443 | | 26.449 | 14.756 | 46.527 | | 18.84 |
| ATOM | 16293 | CG2 | VAL | 2443 | | 27.797 | 16.855 | 46.235 | | 20.62 |
| ATOM | 16294 | C | VAL | 2443 | | 28.743 | 13.675 | 48.162 | | 18.17 |
| | | 0 | VAL | 2443 | | 28.939 | 12.918 | 47.214 | | 18.72 |
| ATOM | 16295 | N | | 2443 | | 28.759 | 13.278 | 49.432 | | 17.59 |
| MOTA | 16296 | | GLY | | | | | | | |
| ATOM | 16297 | CA | GLY | 2444 | | 29.047 | 11.901 | 49.773 | | 17.73 |
| ATOM | 16298 | С | GLY | 2444 | | 27.848 | 11.015 | 50.003 | | 19.75 |
| ATOM | 16299 | 0 | GLY | 2444 | | 26.722 | 11.499 | 50.162 | | 18.97 |
| ATOM | 16300 | N | ASP | 2445 | | 28.083 | 9.706 | 50.019 | | 19.18 |
| MOTA | 16301 | CA | ASP | 2445 | | 26.982 | 8.794 | 50.239 | | 18.23 |
| MOTA | 16302 | CB | ASP | 2445 | | 27.330 | 7.359 | 49.806 | | 20.29 |
| MOTA | 16303 | CG | | 2445 | | 28.573 | 6.810 | 50.478 | | 22.01 |
| ATOM | 16304 | | ASP | 2445 | | 29.074 | 7.424 | 51.443 | | 22.09 |
| MOTA | 16305 | | ASP | 2445 | | 29.039 | 5.741 | 50.030 | | 23.26 |
| MOTA | 16306 | С | ASP | 2445 | | 26.531 | 8.835 | 51.693 | | 17.90 |
| MOTA | 16307 | 0 | ASP | 2445 | | 25.646 | 8.079 | 52.095 | | 12.82 |
| MOTA | 16308 | N | SER | 2446 | | 27.136 | 9.717 | 52.493 | | 16.02 |
| ATOM | 16309 | CA | SER | 2446 | | 26.710 | 9.842 | 53.884 | | 14.42 |
| ATOM | 16310 | CB | SER | 2446 | | 27.556 | 10.877 | 54.632 | | 17.31 |
| MOTA | 16311 | OG | SER | 2446 | | 27.690 | 12.075 | 53.886 | | 19.20 |
| ATOM | 16312 | C | SER | 2446 | | 25.260 | 10.294 | 53.838 | | 13.92 |
| MOTA | 16313 | 0 | SER | 2446 | | 24.510 | 10.114 | 54.799 | | 15.62 |
| MOTA | 16314 | N | LEU | 2447 | | 24.879 | 10.885 | 52.706 | 1.00 | 13.83 |
| MOTA | 16315 | CA | LEU | 2447 | | 23.511 | 11.366 | 52.490 | 1.00 | 15.03 |
| MOTA | 16316 | CB | LEU | 2447 | | 23.383 | 12.005 | 51.095 | 1.00 | 13.29 |
| MOTA | 16317 | CG | LEU | 2447 | | 23.435 | 11.139 | 49.828 | 1.00 | 14.14 |
| MOTA | 16318 | CD1 | LEU | 2447 | | 22.038 | 10.529 | 49.557 | 1.00 | 14.78 |
| MOTA | 16319 | CD2 | LEU | 2447 | | 23.856 | 11.983 | 48.647 | 1.00 | 14.51 |
| MOTA | 16320 | C | LEU | 2447 | | 22.505 | 10.232 | 52.636 | 1.00 | 16.55 |
| MOTA | 16321 | 0 | LEU | 2447 | | 21.325 | 10.464 | 52.923 | 1.00 | 16.84 |
| ATOM | 16322 | N | GLY | 2448 | | 22.974 | 9.003 | 52.433 | 1.00 | 14.34 |
| ATOM | 16323 | CA | GLY | 2448 | | 22.092 | 7.856 | 52.549 | 1.00 | 16.03 |
| ATOM | 16324 | С | GLY | 2448 | | 21.544 | 7.753 | 53.952 | 1.00 | 16.17 |
| MOTA | 16325 | 0 | GLY | 2448 | | 20.468 | 7.212 | 54.170 | 1.00 | 14.30 |
| MOTA | 16326 | N | MET | 2449 | | 22.290 | 8.287 | 54.910 | 1.00 | 16.60 |
| MOTA | 16327 | . CA | MET | 2449 | | 21.872 | 8.245 | 56.292 | 1.00 | 16.34 |
| MOTA | 16328 | CB | MET | 2449 | | 23.056 | 7.814 | 57.157 | 1.00 | 19.82 |
| MOTA | 16329 | CG | MET | 2449 | | 23.644 | 6.484 | 56.710 | 1.00 | 21.64 |
| ATOM | 16330 | SD | MET | 2449 | | 24.990 | 5.908 | 57.750 | 1.00 | 24.22 |
| ATOM | 16331 | CE | MET | 2449 | | 24.077 | 5.356 | 59.175 | 1.00 | 25.30 |
| ATOM | 16332 | С | MET | 2449 | | 21.337 | 9.602 | 56.739 | 1.00 | 17.00 |
| ATOM | 16333 | 0 | MET | 2449 | | 20.194 | 9.710 | 57.177 | 1.00 | 17.40 |
| ATOM | 16334 | N | THR | 2450 | | 22.158 | 10.636 | 56.599 | 1.00 | 16.35 |
| ATOM | 16335 | CA | THR | 2450 | | 21.774 | 11.980 | 57.007 | 1.00 | 18.67 |
| ATOM | 16336 | CB | THR | 2450 | | 22.988 | 12.932 | 56.910 | 1.00 | 20.10 |
| ATOM | 16337 | OG1 | THR | 2450 | | 22.658 | 14.201 | 57.489 | 1.00 | 27.83 |
| ATOM | 16338 | CG2 | THR | 2450 | | 23.394 | 13.137 | 55.468 | 1.00 | 22.03 |
| MOTA | 16339 | С | THR | 2450 | | 20.588 | 12.575 | 56.235 | 1.00 | 18.18 |
| ATOM | 16340 | 0 | THR | 2450 | | 19.764 | 13.287 | 56.808 | 1.00 | 16.73 |
| ATOM | 16341 | N | VAL | 2451 | | 20.487 | 12.277 | 54.943 | 1.00 | 16.56 |
| ATOM | 16342 | CA | VAL | 2451 | | 19.388 | 12.809 | 54.138 | | 15.70 |
| ATOM | 16343 | CB | VAL | 2451 | | 19.904 | 13.319 | 52.771 | | 16.21 |
| MOTA | 16344 | | VAL | 2451 | | 18.737 | 13.687 | 51.857 | | 18.82 |
| ATOM | 16345 | | VAL | 2451 | | 20.794 | 14.531 | 52.983 | | 18.81 |
| ATOM | 16346 | C | VAL | 2451 | | 18.245 | 11.820 | 53.906 | | 15.14 |
| ATOM | 16347 | Ö | VAL | 2451 | - | 17.073 | 12.131 | 54.168 | | 13.37 |
| ATOM | 16348 | N | GLN | 2452 | | 18.580 | 10.631 | 53.415 | | 14.84 |
| MOTA | 16349 | CA | GLN | 2452 | | 17.573 | 9.605 | 53.135 | | 15.81 |
| ATOM | 16350 | CB | GLN | 2452 | | 18.130 | 8.588 | 52.137 | | 11.46 |
| ATOM | 16351 | CG | GLN | 2452 | | 18.666 | 9.217 | 50.868 | | 14.21 |
| MOTA | 16352 | CD | GLN | 2452 | | 19.187 | 8.181 | 49.893 | | 10.70 |
| | | | | | | | | | | |

| ATOM | 16353 | OE1 | GLN | 2452 | 19.456 | 7.044 | 50.279 | 1.00 14.39 |
|------|-------|------|-----|--------|--------|--------|--------|-----------------|
| | | | | 2452 | 19.335 | 8.568 | 48.627 | 1.00 12.31 |
| MOTA | 16354 | NE2 | GLN | | | | | |
| MOTA | 16355 | С | GLN | 2452 | 17.071 | 8.883 | 54.376 | 1.00 15.31 |
| ATOM | 16356 | 0 | GLN | 2452 | 15.931 | 8.424 | 54.412 | 1.00 16.95 |
| ATOM | 16357 | N | GLY | 2453 | 17.919 | 8.760 | 55.392 | 1.00 16.51 |
| | | | | | | | | |
| MOTA | 16358 | CA | GLY | 2453 | 17.480 | 8.111 | 56.619 | - |
| ATOM | 16359 | C | GLY | 2453 | 17.695 | 6.616 | 56.735 | 1.00 16.27 |
| ATOM | 16360 | 0 | GLY | 2453 | 17.069 | 5.961 | 57.567 | 1.00 15.67 |
| | | | | 2454 | 18.576 | 6.070 | 55.903 | 1.00 17.26 |
| MOTA | 16361 | N | HIS | | | | | |
| MOTA | 16362 | CA | HIS | 2454 | 18.878 | 4.638 | 55.945 | 1.00 16.67 |
| MOTA | 16363 | CB | HIS | 2454 | 19.485 | 4.188 | 54.616 | 1.00 16.80 |
| ATOM | 16364 | CG | HIS | 2454 | 18.521 | 4.210 | 53.477 | 1.00 17.61 |
| | | | | | | | | |
| MOTA | 16365 | | HIS | 2454 | 18.472 | 4.977 | 52.363 | 1.00 17.85 |
| ATOM | 16366 | ND1 | HIS | 2454 | 17.454 | 3.344 | 53.396 | 1.00 16.86 |
| ATOM | 16367 | CE1 | HIS | 2454 | 16.790 | 3.573 | 52.278 | 1.00 19.45 |
| | | | | 2454 | 17.387 | 4.559 | 51.633 | 1.00 18.52 |
| ATOM | 16368 | NE2 | | | | | | |
| MOTA | 16369 | С | HIS | 2454 | 19.873 | 4.349 | 57.062 | 1.00 17.34 |
| ATOM | 16370 | 0 | HIS | 2454 | 20.558 | 5.255 | 57.533 | 1.00 18.36 |
| ATOM | 16371 | N | ASP | 2455 | 19.945 | 3.084 | 57.475 | 1.00 18.16 |
| | | | | | | | 58.531 | 1.00 21.37 |
| MOTA | 16372 | CA | ASP | 2455 | 20.858 | 2.646 | | |
| MOTA | 16373 | CB | ASP | 2455 | 20.435 | 1.270 | 59.074 | 1.00 25.85 |
| MOTA | 16374 | CG | ASP | 2455 | 20.380 | 0.193 | 57.991 | 1.00 30.92 |
| MOTA | 16375 | | ASP | 2455 | 21.371 | 0.020 | 57.251 | 1.00 33.11 |
| | | | | | | | | |
| MOTA | 16376 | | ASP | 2455 | 19.344 | -0.496 | 57.883 | 1.00 35.21 |
| MOTA | 16377 | С | ASP | 2455 | 22.315 | 2.561 | 58.061 | 1.00 20.40 |
| MOTA | 16378 | 0 | ASP | 2455 | 23.214 | 2.291 | 58.857 | 1.00 22.38 |
| | | | SER | 2456 | 22.542 | 2.782 | 56.775 | 1.00 19.74 |
| MOTA | 16379 | N | | | | | | |
| MOTA | 16380 | CA · | SER | 2456 | 23.885 | 2.725 | 56.216 | 1.00 19.12 |
| ATOM | 16381 | CB | SER | 2456 | 24.308 | 1.266 | 55.985 | 1.00 20.10 |
| ATOM | 16382 | OG | SER | 2456 | 23.643 | 0.697 | 54.870 | 1.00 21.89 |
| | | | | | | | | |
| MOTA | 16383 | C | SER | 2456 | 23.918 | 3.497 | 54.905 | 1.00 17.48 |
| ATOM | 16384 | 0 | SER | 2456 | 22.893 | 3.985 | 54.440 | 1.00 17.06 |
| ATOM | 16385 | N | THR | 2457 ´ | 25.101 | 3.616 | 54.312 | 1.00 14.78 |
| | | CA | THR | 2457 | 25.245 | 4.342 | 53.057 | 1.00 13.35 |
| MOTA | 16386 | | | | | | | |
| MOTA | 16387 | CB | THR | 2457 | 26.641 | 4.990 | 52.951 | 1.00 14.64 |
| MOTA | 16388 | OG1 | THR | 2457 | 27.623 | 3.973 | 52.751 | 1.00 14.31 |
| ATOM | 16389 | CG2 | THR | 2457 | 26.984 | 5.744 | 54.237 | 1.00 15.15 |
| | | | | | | | | |
| MOTA | 16390 | С | THR | 2457 | 25.050 | 3.469 | 51.816 | 1.00 12.59 |
| ATOM | 16391 | 0 | THR | 2457 | 24.984 | 3.980 | 50.700 | 1.00 14.58 |
| ATOM | 16392 | N | LEU | 2458 | 24.977 | 2.158 | 52.008 | 1.00 13.46 |
| | | | | | | 1.230 | 50.880 | 1.00 15.15 |
| MOTA | 16393 | CA | LEU | 2458 | 24.836 | | | |
| MOTA | 16394 | CB | LEU | 2458 | 24.789 | -0.210 | 51.399 | 1.00 16.30 |
| ATOM | 16395 | CG | LEU | 2458 | 26.150 | -0.857 | 51.711 | 1.00 18.84 |
| | 16396 | | LEU | 2458 | 26.834 | -0.141 | 52.881 | 1.00 18.45 |
| ATOM | | | | | | | | |
| MOTA | 16397 | CD2 | LEU | 2458 | 25.933 | -2.323 | 52.036 | 1.00 19.18 |
| MOTA | 16398 | C | LEU | 2458 | 23.682 | 1.454 | 49.894 | 1.00 16.48 |
| ATOM | 16399 | 0 | LEU | 2458 | 23.853 | 1.265 | 48.690 | 1.00 16.20 |
| | | | | 2459 | 22.496 | 1.843 | 50.388 | 1.00 17.41 |
| MOTA | 16400 | N | PRO | | | | | |
| MOTA | 16401 | CD | PRO | 2459 | 22.096 | 1.948 | 51.801 | 1.00 17.56 |
| ATOM | 16402 | CA | PRO | 2459 | 21.352 | 2.073 | 49.494 | 1.00 16.65 |
| MOTA | 16403 | CB | PRO | 2459 | 20.189 | 2.296 | 50.468 | 1.00 19.49 |
| | | | | | | 2.806 | 51.710 | 1.00 23.52 |
| MOTA | 16404 | CG | PRO | 2459 | 20.870 | | | |
| MOTA | 16405 | C | PRO | 2459 | 21.524 | 3.224 | 48.504 | $1.00^{-1}6.06$ |
| MOTA | 16406 | 0 | PRO | 2459 | 20.800 | 3.311 | 47.511 | 1.00 13.44 |
| ATOM | 16407 | N | VAL | 2460 | 22.486 | 4.105 | 48.766 | 1.00 13.48 |
| | | | | 2460 | 22.725 | 5.239 | 47.882 | 1.00 14.40 |
| MOTA | 16408 | CA | VAL | | | | | |
| MOTA | 16409 | CB | VAL | 2460 | 23.795 | 6.192 | 48.450 | 1.00 14.61 |
| ATOM | 16410 | CG1 | VAL | 2460 | 24.065 | 7.299 | 47.458 | 1.00 14.36 |
| ATOM | 16411 | | VAL | 2460 | 23.329 | 6.762 | 49.780 | 1.00 13.84 |
| | | | | | | 4.789 | | 1.00 15.33 |
| ATOM | 16412 | С | VAL | 2460 | 23.201 | | 46.511 | |
| MOTA | 16413 | Ο. | VAL | 2460 | 24.202 | 4.080 | 46.397 | 1.00 14.73 |
| MOTA | 16414 | N | THR | 2461 | 22.495 | 5.195 | 45.466 | 1.00 16.85 |
| ATOM | 16415 | CA | THR | 2461 | 22.921 | 4.803 | 44.139 | 1.00 19.10 |
| | | | | | | | | |
| MOTA | 16416 | CB | THR | 2461 | 21.798 | 3.984 | 43.403 | 1.00 24.26 |
| MOTA | 16417 | OG1 | THR | 2461 | 20.513 | 4.292 | 43.952 | 1.00 25.02 |
| ATOM | 16418 | CG2 | THR | 2461 | 22.022 | 2.478 | 43.616 | 1.00 25.84 |
| | | | | 2461 | 23.450 | 6.011 | 43.351 | 1.00 18.53 |
| MOTA | 16419 | C | THR | | | | | |
| MOTA | 16420 | 0 | THR | 2461 | 23.338 | 7.153 | 43.802 | 1.00 17.30 |
| ATOM | 16421 | N | VAL | 2462 | 24.074 | 5.758 | 42.207 | 1.00 16.22 |
| ATOM | 16422 | CA | VAL | 2462 | 24.651 | 6.823 | 41.392 | 1.00 16.40 |
| | | | | | | | | |
| ATOM | 16423 | CB | VAL | 2462 | 25.214 | 6.253 | 40.072 | 1.00 15.77 |
| ATOM | 16424 | CG1 | VAL | 2462 | 25.794 | 7.369 | 39.219 | 1.00 15.65 |
| ATOM | 16425 | CG2 | VAL | 2462 | 26.275 | 5.213 | 40.385 | 1.00 18.55 |
| | | | VAL | 2462 | 23.679 | 7.951 | 41.057 | 1.00 16.36 |
| ATOM | 16426 | C | | | | | | |
| ATOM | 16427 | 0 | VAL | 2462 | 24.061 | 9.127 | 41.020 | 1.00 16.32 |
| ATOM | 16428 | N | ALA | 2463 | 22.425 | 7.594 | 40.804 | 1.00 14.77 |
| ATOM | 16429 | CA | ALA | 2463 | 21.417 | 8.586 | 40.475 | 1.00 15.24 |
| | 10127 | CFI | | | , | 2.500 | | |
| | | | | | | | | |

| ATOM | 16430 | CB | ALA | 2463 | 20.100 | 7.900 | 40.118 | 1.00 17.40 |
|--------------|----------------|---------|-------------|--------------|------------------|------------------|------------------|--------------------------|
| ATOM | 16431 | C | ALA | 2463 | 21.211 | 9.540 | 41.647 | 1.00 15.53 |
| ATOM | 16432 | ō | ALA | 2463 | 20.998 | 10.737 | 41.448 | 1.00 17.50 |
| ATOM | 16433 | N | ASP | 2464 | 21.260 | 9.009 | 42.864 | 1.00 15.85 |
| ATOM | 16434 | CA | ASP | 2464 | 21.096 | 9.837 | 44.051 | 1.00 15.44 |
| ATOM | 16435 | CB | ASP | 2464 | 21.161 | 8.999 | 45.338 | 1.00 15.36 |
| MOTA | 16436 | CG | ASP | 2464 | 19.964 | 8.076 | 45.514 | 1.00 16.71 |
| MOTA | 16437 | | ASP | 2464 | 18.885 | 8.353 | 44.930 | 1.00 13.53 |
| MOTA | 16438 | | ASP | 2464 | 20.110 | 7.088 | 46.266 | 1.00 15.10 |
| ATOM | 16439 | С | ASP | 2464 | 22.229 | 10.859 | 44.078 | 1.00 15.31 |
| MOTA | 16440 | 0 | ASP | 2464 | 22.000 | 12.058 | 44.249 | 1.00 14.61 |
| ATOM | 16441 | N | ILE | 2465 | 23.460 | 10.384 | 43.910 | 1.00 14.73 |
| MOTA | 16442 | CA | ILE | 2465 | 24.613 | 11.283 | 43.928 | 1.00 14.21 |
| MOTA | 16443 | CB | ILE | 2465 | 25.937 | 10.504 | 43.708 | 1.00 14.08 |
| MOTA | 16444 | CG2 | ILE | 2465 | 27.104 | 11.484 | 43.609 | 1.00 12.92 |
| MOTA | 16445 | CG1 | ILE | 2465 | 26.159 | 9.511 | 44.861 | 1.00 11.78 |
| MOTA | 16446 | CD1 | ILE | 2465 | 26.437 | 10.163 | 46.224 | 1.00 16.30 |
| MOTA | 16447 | С | ILE | 2465 | 24.482 | 12.377 | 42.867 | 1.00 14.68 |
| MOTA | 16448 | 0 | ILE | 2465 | 24.675 | 13.556 | 43.159 | 1.00 15.78 |
| MOTA | 16449 | N | ALA | 2466 | 24.137 | 11.995 | 41.642 | 1.00 13.89 |
| MOTA | 16450 | CA | ALA | 2466 | 23.993 | 12.960 | 40.551 | 1.00 14.00 |
| MOTA | 16451 | CB | ALA | 2466 | 23.631 | 12.229 | 39.246 | 1.00 13.36 |
| MOTA | 16452 | С | ALA | 2466 | 22.942 | 14.027 | 40.849 | 1.00 14.38 |
| MOTA | 16453 | 0 | ALA | 2466 | 23.082 | 15.179 | 40.445 | 1.00 16.13 |
| MOTA | 16454 | N | TYR | 2467 | 21.871 | 13.620 | 41.518 | 1.00 15.16 |
| MOTA | 16455 | CA | TYR | 2467 | 20.792 | 14.527 | 41.874 | 1.00 14.44 |
| MOTA | 16456 | CB | TYR | 2467 | 19.660 | 13.744 | 42.536 | 1.00 15.27 |
| MOTA | 16457 | CG | TYR | 2467 | 18.537 | 14.592 | 43.094 | 1.00 16.93 |
| MOTA | 16458 | CD1 | TYR | 2467 | 17.661 | 15.271 | 42.252 | 1.00 17.28 |
| MOTA | 16459 | CE1 | TYR | 2467 | 16.603 | 16.016 | 42.765 | 1.00 17.30 |
| ATOM | 16460 | CD2 | TYR | 2467 | 18.331 | 14.680 | 44.471 | 1.00 17.80 |
| MOTA | 16461 | CE2 | TYR | 2467 | 17.281 | 15.419 16.084 | 45.000 44.143 | 1.00 17.99 1.00 19.01 |
| MOTA | 16462 | CZ | TYR | 2467 2467 | 16.415 15.355 | 16.787 | 44.143 | 1.00 19.01 |
| ATOM ATOM | 16463 16464 | C OH | TYR TYR | 2467 | 21.293 | 15.606 | 42.833 | 1.00 10.00 |
| ATOM | 16465 | 0 | TYR | 2467 | 21.094 | 16.799 | 42.605 | 1.00 12.33 |
| ATOM | 16466 | N | HIS | 2468 | 21.942 | 15.180 | 43.905 | 1.00 13.09 |
| ATOM | 16467 | CA | HIS | 2468 | 22.450 | 16.117 | 44.897 | 1.00 14.34 |
| ATOM | 16468 | CB | HIS | 2468 | 22.822 | 15.360 | 46.174 | 1.00 13.15 |
| ATOM | 16469 | CG | HIS | 2468 | 21.632 | 14.846 | 46.924 | 1.00 17.11 |
| ATOM | 16470 | | HIS | 2468 | 21.090 | 13.606 | 46.999 | 1.00 17.53 |
| ATOM | 16471 | | HIS | 2468 | 20.797 | 15.671 | 47.649 | 1.00 15.01 |
| ATOM | 16472 | | HIS | 2468 | 19.792 | 14.963 | 48.134 | 1.00 17.40 |
| ATOM | 16473 | NE2 | | 2468 | 19.945 | 13.707 | 47.753 | 1.00 18.53 |
| MOTA | 16474 | С | HIS | 2468 | 23.626 | 16.936 | 44.378 | 1.00 15.33 |
| ATOM | 16475 | 0 | HIS | 2468 | 23.834 | 18.069 | 44.803 | 1.00 14.82 |
| ATOM | 16476 | N | THR | 2469 | 24.391 | 16.366 | 43.452 | 1.00 15.33 |
| ATOM | 16477 | CA | THR | 2469 | 25.527 | 17.073 | 42.873 | 1.00 16.60 |
| ATOM | 16478 | CB | THR | 2469 | 26.348 | 16.132 | 41.968 | 1.00 16.20 |
| MOTA | 16479 | OG1 | THR | 2469 | 27.046 | 15.184 | 42.785 | 1.00 17.12 |
| MOTA | 16480 | CG2 | THR | 2469 | 27.352 | 16.919 | 41.134 | 1.00 14.14 |
| MOTA | 16481 | C | THR | 2469 | 25.066 | 18.298 | 42.078 | 1.00 16.62 |
| MOTA | 16482 | 0 | THR | 2469 | 25.631 | 19.387 | 42.215 | 1.00 18.28 |
| MOTA | 16483 | N | ALA | 2470 | 24.034 | 18.122 | 41.256 | 1.00 17.01 |
| ATOM | 16484 | CA | ALA | 2470 | 23.508 | 19.222 | 40.461 | 1.00 16.73 |
| MOTA | 16485 | CB | ALA | 2470 | 22.383 | 18.726 | 39.549 | 1.00 18.75 |
| MOTA | 16486 | С | ALA | 2470 | 22.992 | 20.320 | 41.391 | 1.00 17.94 |
| ATOM | 16487 | 0 | ALA | 2470 | 23.185 | 21.505 | 41.125 | 1.00 18.99 |
| ATOM | 16488 | N | ALA | 2471 | 22.342 | 19.921 | 42.479 | 1.00 17.24 |
| ATOM | 16489 | CA | ALA | 2471 | 21.807 | 20.875 | 43.445 | 1.00 19.28 |
| ATOM | 16490 | CB | ALA | 2471 | 21.024 | 20.137 | 44.529 44.083 | 1.00 18.10 |
| MOTA | 16491 | C | ALA | 2471 | 22.921 | 21.705 | | 1.00 20.30 |
| ATOM | 16492 16493 | O N | ALA Vat. | 2471 | 22.814 23.987 | 22.927 21.036 | 44.191 44.510 | 1.00 22.29 1.00 21.49 |
| MOTA MOTA | 16493 | N CA | VAL VAL | 2472 2472 | 25.126 | 21.036 | 44.510 | 1.00 21.49 |
| ATOM | 16494 | CB | VAL | 2472 | 26.149 | 20.670 | 45.669 | 1.00 20.38 |
| ATOM | 16496 | | VAL | 2472 | 27.441 | 21.359 | 46.104 | 1.00 20.42 |
| ATOM | 16497 | | VAL | 2472 | 25.543 | 19.901 | 46.832 | 1.00 17.07 |
| MOTA | 16498 | C | VAL | 2472 | 25.829 | 22.656 | 44.178 | 1.00 21.47 |
| MOTA | 16499 | 0 | VAL | 2472 | 26.220 | 23.763 | 44.552 | 1.00 20.66 |
| ATOM | 16500 | N | ARG | 2473 | 26.000 | 22.215 | 42.938 | 1.00 20.73 |
| MOTA | 16501 | CA | ARG | 2473 | 26.651 | 23.043 | 41.939 | 1.00 20.95 |
| ATOM | 16502 | CB | ARG | 2473 | 26.805 | 22.273 | 40.622 | 1.00 21.67 |
| MOTA | 16503 | CG | ARG | 2473 | 27.384 | 23.113 | 39.490 | 1.00 23.02 |
| MOTA | 16504 | CD | ARG | 2473 | 28.729 | 23.711 | 39.889 | 1.00 23.89 |
| MOTA | 16505 | NE | ARG | 2473 | 29.797 | 22.724 | 39.904 | 1.00 23.45 |
| MOTA | 16506 | CZ | ARG | 2473 | 30.932 | 22.858 | 40.584 | 1.00 26.20 |

| | ATOM | 16507 | NILI 1 | ARG | 2473 | 31.148 | 23.941 | 41.320 | 1.00 24.63 |
|---|--------------------------------------|----------------------------------|-----------|-------------------|----------------------|----------------------------|----------------------------|----------------------------|--|
| | | 16508 | NH2 | ARG | 2473 | 31.864 | 21.915 | 40.515 | 1.00 21.81 |
| | ATOM | | | | | | | | |
| | ATOM | 16509 | C | ARG | 2473 | 25.857 | 24.326 | 41.699 | 1.00 22.12 |
| | MOTA | 16510 | 0 | ARG | 2473 | 26.437 | 25.398 | 41.529 | 1.00 23.41 |
| | ATOM | 16511 | N | ARG | 2474 | 24.532 | 24.229 | 41.684 | 1.00 20.61 |
| | ATOM | 16512 | CA | ARG | 2474 | 23.728 | 25.424 | 41.459 | 1.00 22.05 |
| | ATOM | 16513 | CB | ARG | 2474 | 22.237 | 25.075 | 41.369 | 1.00 23.15 |
| | ATOM | 16514 | CG | ARG | 2474 | 21.883 | 24.197 | 40.178 | 1.00 25.72 |
| | | | | | 2474 | 20.381 | 24.163 | 39.933 | 1.00 26.31 |
| | ATOM | 16515 | CD | ARG | | | | | |
| | ATOM | 16516 | NE | ARG | 2474 | 20.023 | 23.166 | 38.930 | 1.00 29.12 |
| | ATOM | 16517 | CZ | ARG | 2474 | 19.951 | 21.859 | 39.159 | 1.00 30.89 |
| | ATOM | 16518 | NH1 | ARG | 2474 | 20.205 | 21.375 | 40.370 | 1.00 31.05 |
| | MOTA | 16519 | NH2 | ARG | 2474 | 19.638 | 21.030 | 38.168 | 1.00 29.85 |
| | MOTA | 16520 | С | ARG | 2474 | 23.958 | 26.446 | 42.571 | 1.00 21.79 |
| | ATOM | 16521 | ō | ARG | 2474 | 23.888 | 27.651 | 42.337 | 1.00 19.95 |
| | ATOM | 16522 | N | GLY | 2475 | 24.249 | 25.959 | 43.772 | 1.00 21.36 |
| | | | | | | | | | |
| | ATOM | 16523 | CA | GLY | 2475 | 24.487 | 26.853 | 44.889 | 1.00 23.25 |
| | MOTA | 16524 | С | GLY | 2475 | 25.922 | 27.337 | 44.982 | 1.00 23.98 |
| | ATOM | 16525 | 0 | GLY | 2475 | 26.186 | 28.396 | 45.552 | 1.00 23.43 |
| | ATOM | 16526 | N | ALA | 2476 | 26.849 | 26.568 | 44.418 | 1.00 23.91 |
| | MOTA | 16527 | CA | ALA | 2476 | 28.264 | 26.920 | 44.447 | 1.00 25.38 |
| | ATOM | 16528 | CB | ALA | 2476 | 28.948 | 26.219 | 45.616 | 1.00 25.54 |
| | ATOM | 16529 | c | ALA | 2476 | 28.930 | 26.517 | 43.134 | 1.00 26.02 |
| | ATOM | 16530 | ō | ALA | 2476 | 29.616 | 25.498 | 43.066 | 1.00 27.80 |
| | | | | | | | | | |
| | ATOM | 16531 | N | PRO | 2477 | 28.741 | 27.319 | 42.074 | 1.00 26.85 |
| | ATOM | 16532 | CD | PRO | 2477 | 27.952 | 28.563 | 42.035 | 1.00 28.05 |
| | MOTA | 16533 | CA | PRO | 2477 | 29.322 | 27.038 | 40.757 | 1.00 29.05 |
| | MOTA | 16534 | CB | PRO | 2477 | 28.607 | 28.035 | 39.853 | 1.00 28.77 |
| | MOTA | 16535 | CG | PRO | 2477 | 28.429 | 29.204 | 40.748 | 1.00 29.67 |
| | ATOM | 16536 | C | PRO | 2477 | 30.839 | 27.159 | 40.664 | 1.00 29.31 |
| | ATOM | 16537 | ō | PRO | 2477 | 31.441 | 26.680 | 39.706 | 1.00 30.76 |
| | | | | | | | | | |
| | ATOM | 16538 | N | ASN | 2478 | 31.453 | 27.788 | 41.661 | 1.00 30.39 |
| | ATOM | 16539 | CA | ASN | 2478 | 32.897 | 27.974 | 41.655 | 1.00 29.62 |
| | MOTA | 16540 | CB | ASN | 2478 | 33.229 | 29.453 | 41.881 | 1.00 30.92 |
| | MOTA | 16541 | CG | ASN | 2478 | 32.571 | 30.360 | 40.858 | 1.00 31.62 |
| | ATOM | 16542 | OD1 | ASN | 2478 | 32.859 | 30.284 | 39.665 | 1.00 33.22 |
| | ATOM | 16543 | ND2 | ASN | 2478 | 31.667 | 31.215 | 41.322 | 1.00 34.26 |
| | ATOM | 16544 | С | ASN | 2478 | 33.616 | 27.128 | 42.695 | 1.00 28.50 |
| | ATOM | 16545 | ō | ASN | 2478 | 34.828 | 27.231 | 42.842 | 1.00 29.41 |
| | | | | | | | | | |
| | MOTA | 16546 | N | CYS | 2479 | 32.877 | 26.280 | 43.402 | 1.00.27.76 |
| | MOTA | 16547 | CA | CYS | 2479 | 33.487 | 25.444 | 44.428 | 1.00 24.78 |
| | MOTA | 16548 | CB | CYS | 2479 | 32.444 | 25.031 | 45.475 | 1.00 25.50 |
| | MOTA | 16549 | SG | CYS | 2479 | 31.459 | 23.551 | 45.037 | 1.00 26.02 |
| | MOTA | 16550 | С | CYS | 2479 | 34.122 | 24.188 | 43.845 | 1.00 24.27 |
| | MOTA | 16551 | 0 | CYS | 2479 | 33.787 | 23.760 | 42.740 | 1.00 23.85 |
| | ATOM | 16552 | N | LEU | 2480 | 35.065 | 23.616 | 44.589 | 1.00 22.97 |
| | ATOM | 16553 | CA | LEU | 2480 | 35.697 | 22.375 | 44.175 | 1.00 22.48 |
| | | | | | | | | | |
| | ATOM | 16554 | CB | LEU | 2480 | 37.062 | 22.189 | 44.852 | 1.00 22.33 |
| | MOTA | 16555 | CG | LEU | 2480 | 37.763 | 20.855 | 44.584 | 1.00 23.00 |
| | ATOM | 16556 | CD1 | | 2480 | 37.990 | 20.684 | 43.095 | 1.00 23.31 |
| | MOTA | 16557 | CD2 | LEU | 2480 | 39.087 | 20.787 | 45.335 | 1.00 22.05 |
| | MOTA | 16558 | С | LEU | 2480 | 34.693 | 21.342 | 44.680 | 1.00 21.39 |
| | ATOM | 16559 | 0 | LEU | 2480 | 34.571 | 21.114 | 45.884 | 1.00 20.80 |
| | ATOM | 16560 | N | LEU | 2481 | 33.960 | 20.739 | 43.749 | 1.00 20.74 |
| | ATOM | 16561 | CA | LEU | 2481 | 32.926 | 19.772 | 44.089 | 1.00 19.90 |
| | ATOM | 16562 | CB | LEU | 2481 | 31.684 | 20.025 | 43.217 | 1.00 21.31 |
| | | | | | 2481 | | | | |
| | ATOM | 16563 | CG CD1 | LEU | | 30.295 | 19.607 | 43.726 | 1.00 24.25 |
| | MOTA | 16564 | CD1 | | 2481 | 29.231 | 20.182 | 42.806 | 1.00 24.77 |
| | MOTA | 16565 | CD2 | | 2481 | 30.184 | 18.094 | 43.805 | 1.00 25.65 |
| | MOTA | 16566 | С | LEU | 2481 | 33.384 | 18.328 | 43.931 | 1.00 20.50 |
| | ATOM | 16567 | 0 | LEU | 2481 | 33.681 | 17.875 | 42.824 | 1.00 20.28 |
| | ATOM | 16568 | N | LEU | 2482 | 33.451 | 17.613 | 45.046 | 1.00 19.62 |
| | ATOM | 16569 | | LEU | 2482 | 33.844 | 16.211 | 45.030 | 1.00 19.59 |
| | ATOM | 16570 | CB | LEU | 2482 | 34.776 | 15.889 | 46.198 | 1.00 19.36 |
| | | 16571 | | | | | | | |
| | ATOM | | CG | LEU | 2482 | 36.249 | 16.304 | 46.107 | 1.00 21.46 |
| | MOTA | 16572 | CD1 | | 2482 | 36.385 | 17.805 | 45.908 | 1.00 24.55 |
| | ATOM | 16573 | CD2 | | 2482 | 36.947 | 15.854 | 47.372 | 1.00 19.98 |
| | MOTA | 16574 | С | LEU | 2482 | 32.569 | 15.397 | 45.178 | 1.00 19.82 |
| | MOTA | 16575 | 0 | LEU | 2482 | 31.701 | 15.752 | 45.972 | 1.00 21.78 |
| | ATOM | 16576 | N | ALA | 2483 | 32.432 | 14.323 | 44.411 | 1.00 16.25 |
| | | 16577 | CA | ALA | 2483 | 31.240 | 13.493 | 44.541 | 1.00 16.04 |
| | ATOM | | | | | | | | |
| | ATOM ATOM | | CB | ΔΤ.Δ | 2484 | | | | 1 00 15 47 |
| | ATOM | 16578 | CB | ALA | 2483 | 30.348 | 13.636 | 43.323 | 1.00 15.47 |
| | MOTA MOTA | 16578 16579 | С | ALA | 2483 | 31.678 | 12.051 | 44.714 | 1.00 14.99 |
| | ATOM ATOM ATOM | 16578 16579 16580 | C 0 | ALA ALA | 2483 2483 | 31.678 32.594 | 12.051 11.591 | 44.714 44.039 | 1.00 14.99 1.00 14.48 |
| | ATOM ATOM ATOM ATOM | 16578 16579 16580 16581 | C N | ALA ALA ASP | 2483 2483 2484 | 31.678 32.594 31.033 | 12.051 11.591 11.346 | 44.714 44.039 45.636 | 1.00 14.99 1.00 14.48 1.00 14.00 |
| | ATOM ATOM ATOM ATOM ATOM | 16578 16579 16580 | C 0 | ALA ALA | 2483 2483 | 31.678 32.594 | 12.051 11.591 | 44.714 44.039 | 1.00 14.99 1.00 14.48 |
| - | ATOM ATOM ATOM ATOM | 16578 16579 16580 16581 | C N | ALA ALA ASP | 2483 2483 2484 | 31.678 32.594 31.033 | 12.051 11.591 11.346 | 44.714 44.039 45.636 | 1.00 14.99 1.00 14.48 1.00 14.00 |

| | ATOM | 16584 | CG | ASP | 2484 | 31.751 | 9.800 | 48.420 | 1.00 21.09 |
|---|--|--|---|--|--|--|---|--|--|
| | ATOM | 16585 | | ASP | 2484 | 32.952 | 10.027 | 48.201 | 1.00 23.51 |
| | ATOM | 16586 | | ASP | 2484 | 31.259 | 9.765 | 49.567 | 1.00 25.92 |
| | ATOM | 16587 | C | ASP | 2484 | 30.751 | 8.990 | 44.906 | 1.00 16.88 |
| | ATOM | 16588 | Ō | ASP | 2484 | 29.679 | 9.252 | 44.362 | 1.00 17.02 |
| | ATOM | 16589 | N | LEU | 2485 | 31.437 | 7.878 | 44.664 | 1.00 16.05 |
| | ATOM | 16590 | CA | LEU | 2485 | 30.856 | 6.828 | 43.837 | 1.00 16.81 |
| | ATOM | 16591 | СВ | LEU | 2485 | 31.887 | 6.120 | 42.968 | 1.00 17.36 |
| | ATOM | 16592 | CG | LEU | 2485 | 32.362 | 6.967 | 41.791 | 1.00 18.54 |
| | ATOM | 16593 | | LEU | 2485 | 33.158 | 6.088 | 40.829 | 1.00 19.06 |
| | ATOM | 16594 | | LEU | 2485 | 31.157 | 7.568 | 41.072 | 1.00 18.74 |
| | ATOM | 16595 | С | LEU | 2485 | 30.367 | 5.900 | 44.936 | 1.00 15.90 |
| | ATOM | 16596 | 0 | LEU | 2485 | 31.145 | 5.447 | 45.773 | 1.00 16.45 |
| | ATOM | 16597 | N | PRO | 2486 | 29.057 | 5.638 | 44.970 | 1.00 17.02 |
| | ATOM | 16598 | CD | PRO | 2486 | 28.055 | 6.209 | 44.052 | 1.00 16.98 |
| | MOTA | 16599 | CA | PRO | 2486 | 28.427 | 4.777 | 45.968 | 1.00 15.60 |
| | MOTA | 16600 | CB | PRO | 2486 | 26.937 | 5.042 | 45.750 | 1.00 15.78 |
| | MOTA | 16601 | CG | PRO | 2486 | 26.860 | 5.312 | 44.276 | 1.00 16.02 |
| | MOTA | 16602 | С | PRO | 2486 | 28.778 | 3.287 | 45.908 | 1.00 14.53 |
| | MOTA | 16603 | 0 | PRO | 2486 | 29.499 | 2.822 | 45.025 | 1.00 14.20 |
| | MOTA | 16604 | N | PHE | 2487 | 28.267 | 2.559 | 46.890 | 1.00 14.83 |
| | MOTA | 16605 | CA | PHE | 2487 | 28.469 | 1.125 | 47.011 | 1.00 15.84 |
| | MOTA | 16606 | CB | PHE | 2487 | 27.501 | 0.583 | 48.074 | 1.00 15.61 |
| | MOTA | 16607 | CG | PHE | 2487 | 27.356 | -0.919 | 48.083 | 1.00 17.92 |
| | MOTA | 16608 | | PHE | 2487 | 28.450 | -1.746 | 48.328 | 1.00 16.77 |
| | MOTA | 16609 | | PHE | 2487 | 26.106 | -1.504 | 47.874 | 1.00 15.14 |
| | MOTA | 16610 | | PHE | 2487 | 28.302 | -3.131 | 48.369 | 1.00 18.81 |
| | MOTA | 16611 | | PHE | 2487 | 25.948 | -2.887 | 47.913 | 1.00 18.55 |
| | ATOM | 16612 | CZ | PHE | 2487 | 27.050 | -3.706 | 48.160 | 1.00 17.93 |
| | MOTA | 16613 | С | PHE | 2487 | 28.283 | 0.389 | 45.676 | 1.00 16.50 |
| | MOTA | 16614 | 0 | PHE | 2487 | 27.257 | 0.535 | 45.007 | 1.00 15.22 |
| | MOTA | 16615 | N | MET | 2488 | 29.297 | -0.390 | 45.302 | 1.00 16.30 |
| | ATOM | 16616 | CA | MET | 2488 | 29.305 | -1.193 | 44.077 | 1.00 16.43 |
| | ATOM | 16617 | CB | MET | 2488 | 28.265 | -2.320 | 44.174 | 1.00 17.44 |
| | ATOM | 16618 | CG | MET | 2488 2488 | 28.596 | -3.554 | 43.353 43.921 | 1.00 17.50 1.00 15.86 |
| | ATOM ATOM | 16619 16620 | SD CE | MET. MET | 2488 | 30.158 29.646 | -4.247 -5.320 | 45.243 | 1.00 15.86 |
| | ATOM | 16621 | CE | MET | 2488 | 29.046 | -0.384 | 42.804 | 1.00 15.24 |
| | ATOM | 16622 | 0 | MET | 2488 | 28.516 | -0.384 | 41.827 | 1.00 18.13 |
| | ATOM | 16623 | N | ALA . | | 29.547 | 0.862 | 42.810 | 1.00 17.32 |
| | ATOM | 16624 | CA | ALA | 2489 | 29.417 | 1.732 | 41.643 | 1.00 16.90 |
| | ATOM | 16625 | CB | ALA | 2489 | 28.963 | 3.133 | 42.074 | 1.00 15.45 |
| | ATOM | 16626 | C | ALA | 2489 | 30.750 | 1.807 | 40.891 | 1.00 14.87 |
| | ATOM | 16627 | ō | ALA | 2489 | 30.887 | 2.539 | 39.916 | 1.00 16.09 |
| | ATOM | 16628 | N | TYR | 2490 | 31.731 | 1.040 | 41.352 | 1.00 16.77 |
| | ATOM | 16629 | CA | TYR | 2490 | 33.043 | 1.000 | 40.705 | 1.00 16.61 |
| | ATOM | 16630 | CB | TYR | 2490 | 33.978 | 2.071 | 41.293 | 1.00 17.08 |
| | ATOM | 16631 | CG | TYR | 2490 | 34.015 | 2.131 | 42.812 | 1.00 19.16 |
| | MOTA | 16632 | an1 | TYR | 2490 | 25 222 | 1 501 | | |
| | ATOM | | CD1 | | 220 | 35.039 | 1.521 | 43.538 | 1.00 18.38 |
| | MOTA | 16633 | | TYR | 2490 | 35.039 35.062 | 1.572 | 43.538 44.939 | 1.00 18.38 1.00 18.54 |
| | 0 | 16633 16634 | | TYR | | | | | |
| | | | CE1 CD2 | TYR | 2490 | 35.062 | 1.572 | 44.939 43.519 44.907 | 1.00 18.54 1.00 20.42 1.00 20.22 |
| | | 16634 | CE1 CD2 CE2 CZ | TYR TYR | 2490 2490 | 35.062 33.011 33.017 34.042 | 1.572 2.795 2.855 2.244 | 44.939 43.519 44.907 45.613 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 21.20 |
| | ATOM . | 16634 16635 16636 16637 | CE1 CD2 CE2 | TYR TYR TYR TYR TYR | 2490 2490 2490 2490 2490 | 35.062 33.011 33.017 34.042 34.038 | 1.572 2.795 2.855 2.244 2.326 | 44.939 43.519 44.907 45.613 46.990 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 21.20 1.00 19.10 |
| | ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16638 | CE1 CD2 CE2 CZ OH C | TYR TYR TYR TYR TYR TYR | 2490 2490 2490 2490 2490 2490 | 35.062 33.011 33.017 34.042 34.038 33.652 | 1.572 2.795 2.855 2.244 2.326 -0.390 | 44.939 43.519 44.907 45.613 46.990 40.875 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 21.20 1.00 19.10 1.00 16.36 |
| | ATOM . ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16638 16639 | CE1 CD2 CE2 CZ OH C | TYR TYR TYR TYR TYR TYR TYR TYR | 2490 2490 2490 2490 2490 2490 2490 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 21.20 1.00 19.10 1.00 16.36 1.00 15.49 |
| | ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16638 16639 16640 | CE1 CD2 CE2 CZ OH C | TYR TYR TYR TYR TYR TYR TYR TYR TYR ALA | 2490 2490 2490 2490 2490 2490 2490 2491 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.687 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 21.20 1.00 19.10 1.00 16.36 1.00 15.49 1.00 15.34 |
| | ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16638 16639 16640 | CE1 CD2 CE2 CZ OH C O N | TYR TYR TYR TYR TYR TYR TYR TYR ALA ALA | 2490 2490 2490 2490 2490 2490 2490 2491 2491 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.687 40.845 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 21.20 1.00 19.10 1.00 16.36 1.00 15.49 1.00 15.34 1.00 16.21 |
| | ATOM ATOM MOTA MOTA MOTA MOTA MOTA MOTA | 16634 16635 16636 16637 16638 16639 16640 16641 16642 | CE1 CD2 CE2 CZ OH C O N CA CB | TYR TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA | 2490 2490 2490 2490 2490 2490 2490 2491 2491 2491 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 32.016 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.687 40.845 40.865 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 21.20 1.00 16.36 1.00 15.49 1.00 15.34 1.00 16.21 1.00 16.00 |
| | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16638 16639 16640 16641 16642 | CE1 CD2 CE2 CZ OH C O N CA CB | TYR TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA | 2490 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 32.016 34.218 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 -3.256 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.687 40.845 40.865 39.765 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 21.20 1.00 19.10 1.00 16.36 1.00 15.49 1.00 15.34 1.00 16.21 1.00 16.00 1.00 16.41 |
| | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16638 16639 16640 16641 16642 16643 | CE1 CD2 CE2 CZ OH C O N CA CB C | TYR TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA ALA ALA | 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 2491 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 32.016 34.218 34.948 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 -3.256 -4.229 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.687 40.845 40.865 39.765 39.945 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 21.20 1.00 19.10 1.00 16.36 1.00 15.49 1.00 16.21 1.00 16.00 1.00 16.41 1.00 16.41 |
| | MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA | 16634 16635 16636 16637 16638 16639 16640 16641 16642 16643 16644 | CE1 CD2 CE2 CZ OH C O N CA CB C O | TYR TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA ALA ALA THR | 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 2491 2491 2492 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 32.016 34.218 34.948 34.196 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 -3.256 -4.229 -2.571 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.687 40.865 39.765 39.945 38.631 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 21.20 1.00 19.10 1.00 16.36 1.00 15.49 1.00 16.21 1.00 16.00 1.00 16.41 1.00 16.54 1.00 16.54 |
| | MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA | 16634 16635 16636 16637 16638 16639 16640 16641 16642 16643 16644 16645 | CE1 CD2 CE2 CZ OH C O N CA CB C O N | TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA ALA THR THR | 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 2491 2491 2492 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 32.016 34.218 34.948 34.196 35.127 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 -3.256 -4.229 -2.571 -2.863 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.687 40.845 40.865 39.765 39.765 39.945 38.631 37.544 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 19.10 1.00 15.49 1.00 15.34 1.00 16.21 1.00 16.41 1.00 16.54 1.00 16.54 1.00 16.89 1.00 18.84 |
| | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16638 16640 16641 16642 16643 16644 16645 16646 | CE1 CD2 CE2 CZ OH C O N CA CB C O N CA | TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA THR THR THR | 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 2491 2492 2492 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 32.016 34.218 34.948 34.196 35.127 34.507 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 -3.256 -4.229 -2.571 -2.863 -3.747 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.687 40.845 39.765 39.765 39.45 39.45 39.45 39.45 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 19.10 1.00 15.49 1.00 15.34 1.00 16.21 1.00 16.00 1.00 16.41 1.00 16.54 1.00 16.89 1.00 18.84 1.00 17.42 |
| | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16638 16640 16641 16642 16643 16644 16645 16646 16647 | CE1 CD2 CE2 CZ OH C O N CA CB C O N CA | TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA THR THR THR | 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 2491 2492 2492 2492 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 32.016 34.218 34.948 34.196 35.127 34.507 33.628 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 -3.256 -4.229 -2.571 -2.863 -3.747 -2.948 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.687 40.845 39.765 39.765 39.945 33.631 37.544 36.423 35.619 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 19.10 1.00 16.36 1.00 15.49 1.00 16.21 1.00 16.00 1.00 16.41 1.00 16.89 1.00 18.84 1.00 18.84 1.00 17.42 1.00 19.01 |
| | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16638 16640 16641 16642 16643 16644 16645 16647 16648 | CE1 CD2 CE2 CZ OH C O N CA CB C O CB CG2 | TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA THR THR THR THR | 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 2491 2492 2492 2492 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 33.240 34.218 34.948 34.196 35.127 34.507 33.628 33.753 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.866 -3.716 -3.256 -4.229 -2.571 -2.863 -3.747 -2.948 -4.919 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.687 40.845 39.765 39.765 39.945 38.631 37.544 36.423 35.619 37.015 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 21.20 1.00 19.10 1.00 16.36 1.00 15.49 1.00 16.21 1.00 16.00 1.00 16.41 1.00 16.54 1.00 16.89 1.00 17.42 1.00 19.01 1.00 19.01 |
| | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16638 16640 16641 16642 16643 16644 16645 16646 16647 16648 | CE1 CD2 CE2 CZ OH C O N CA CB C O CA CB CCA CB | TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA THR THR THR THR THR | 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 2492 2492 2492 2492 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 32.016 34.218 34.948 34.196 35.127 34.507 33.628 33.753 35.476 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 -3.256 -4.229 -2.571 -2.863 -3.747 -2.948 -4.919 -1.517 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.687 40.865 39.765 39.945 38.631 37.544 36.423 37.015 36.939 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 21.20 1.00 19.10 1.00 16.36 1.00 15.49 1.00 16.21 1.00 16.00 1.00 16.41 1.00 16.54 1.00 16.89 1.00 17.42 1.00 19.01 1.00 16.56 1.00 19.00 |
| - | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16638 16640 16641 16642 16644 16645 16647 16647 16649 16650 16651 | CE1 CD2 CE2 CZ OH C O N CA CB C O CB C O CA CB C O C O | TYR TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA THR THR THR THR THR THR | 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 2492 2492 2492 2492 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 32.016 34.948 34.196 35.127 34.507 33.628 33.753 35.476 34.705 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 -3.256 -4.229 -2.571 -2.863 -3.747 -2.948 -4.919 -1.517 -0.563 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.865 39.765 39.765 39.945 38.631 37.544 36.423 35.619 37.015 36.939 37.040 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 19.10 1.00 15.49 1.00 15.34 1.00 16.21 1.00 16.00 1.00 16.41 1.00 16.54 1.00 16.89 1.00 19.20 1.00 19.20 1.00 19.20 1.00 19.20 1.00 19.20 |
| | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16638 16640 16641 16642 16644 16645 16646 16647 16648 16650 16651 16652 | CE1 CD2 CE2 CZ OH C O N CA CB C O N CA CB O CA CB O O N | TYR TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA THR | 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 2492 2492 2492 2492 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 32.016 34.218 34.948 34.196 35.127 34.507 33.628 33.753 35.476 34.705 36.655 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 -3.256 -4.229 -2.571 -2.863 -3.747 -2.948 -4.919 -1.517 -0.563 -1.416 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.687 40.865 39.765 39 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 19.10 1.00 15.49 1.00 15.34 1.00 16.21 1.00 16.41 1.00 16.54 1.00 16.54 1.00 16.54 1.00 16.54 1.00 16.56 1.00 19.01 1.00 16.56 1.00 19.20 1.00 17.78 1.00 20.58 |
| | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16638 16640 16641 16642 16644 16645 16646 16647 16648 16649 16650 16651 16652 | CE1 CD2 CE2 CZ OH C O N CA CB C O CA CB OG1 CG2 C O N CA | TYR TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA THR | 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 2492 2492 2492 2492 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 32.016 34.218 34.948 34.196 35.127 34.507 33.628 33.753 35.476 34.705 36.655 37.710 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 -3.256 -4.229 -2.571 -2.863 -3.747 -2.948 -4.919 -1.517 -0.563 -1.416 -2.440 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.687 40.865 39.765 39.765 39.45 36.423 35.619 37.015 36.939 37.040 36.316 36.217 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 19.10 1.00 19.10 1.00 15.49 1.00 15.34 1.00 16.21 1.00 16.00 1.00 16.41 1.00 16.54 1.00 16.54 1.00 16.56 1.00 19.01 1.00 19.01 1.00 19.02 1.00 19.03 1.00 19.20 1.00 17.78 1.00 20.58 1.00 22.28 |
| | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16638 16640 16641 16642 16643 16644 16645 16646 16647 16648 16649 16650 16651 16652 16653 | CE1 CD2 CE2 CZ OH CO N CA CB C O N CA CB CO O N CA CB OG1 CG2 C O N CD CA | TYR TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA THR THR THR THR THR PRO PRO PRO | 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 2492 2492 2492 2492 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 34.218 34.948 34.196 35.127 34.507 33.628 33.753 35.476 34.705 36.655 37.710 37.080 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 -3.256 -4.229 -2.571 -2.863 -3.747 -2.948 -4.919 -1.517 -0.563 -1.416 -2.440 -0.163 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.687 40.845 40.865 39.765 39.945 38.631 37.544 35.619 37.015 36.939 37.040 36.217 35.696 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 21.20 1.00 19.10 1.00 16.36 1.00 15.49 1.00 16.21 1.00 16.21 1.00 16.41 1.00 16.54 1.00 16.89 1.00 17.42 1.00 19.01 1.00 19.01 1.00 19.02 1.00 17.78 1.00 20.58 1.00 22.28 1.00 21.26 |
| | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16639 16640 16641 16642 16644 16645 16644 16645 16650 16651 16653 16654 16654 | CE1 CD2 CE2 CZ CO OH CO ON CA CB CCB OG1 CG2 C O N CCB CG2 C C CCB CCB CCCA CCB | TYR TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA THR THR THR THR THR PRO PRO PRO | 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 2492 2492 2492 2492 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 32.016 34.218 34.948 34.196 35.127 34.507 33.628 33.753 35.476 34.705 36.655 37.710 37.080 38.359 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 -3.256 -4.229 -2.571 -2.863 -3.747 -2.948 -4.919 -1.517 -0.563 -1.416 -2.440 -0.163 -0.561 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.687 40.845 39.765 39.945 38.631 37.544 36.423 35.619 37.015 36.939 37.040 36.316 36.316 36.316 37.040 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 21.20 1.00 19.10 1.00 16.36 1.00 15.49 1.00 16.21 1.00 16.00 1.00 16.41 1.00 16.54 1.00 16.89 1.00 17.42 1.00 17.42 1.00 19.01 1.00 19.01 1.00 19.01 1.00 17.78 1.00 20.28 1.00 22.28 1.00 22.28 |
| | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16639 16640 16641 16642 16644 16645 16646 16647 16650 16651 16652 16655 16655 | CE1 CD2 CE2 CZ CZ OH CO N CA CB CC CB CC O N CA CB CC | TYR TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA THR THR THR THR THR PRO PRO PRO PRO PRO | 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 2492 2492 2492 2492 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 34.218 34.948 34.196 35.127 34.507 34.507 33.628 33.753 35.476 34.705 36.655 37.710 37.080 38.359 38.925 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 -3.256 -4.229 -2.571 -2.863 -3.747 -2.948 -4.919 -1.517 -0.563 -1.416 -2.440 -0.163 -0.561 -1.615 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.865 39.765 39.945 38.631 37.544 36.423 35.619 37.015 36.939 37.040 36.316 36.217 36.939 37.040 36.316 36.939 37.040 36.316 36.939 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 21.20 1.00 19.10 1.00 16.36 1.00 15.49 1.00 16.21 1.00 16.00 1.00 16.41 1.00 16.54 1.00 16.89 1.00 19.20 1.00 19.01 1.00 19.01 1.00 16.56 1.00 19.20 1.00 17.78 1.00 22.28 1.00 22.28 1.00 22.19 1.00 22.73 |
| | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16639 16640 16641 16642 16644 16645 16647 16646 16650 16651 16652 16653 16655 16655 | CE1 CD2 CE2 CZ CC OH CA CB CA CB CC CB CC | TYR TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA THR THR THR THR THR PRO PRO PRO PRO PRO PRO PRO | 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 2492 2492 2492 2492 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 32.016 34.948 34.196 35.127 34.507 33.628 33.753 35.476 34.705 36.655 37.710 37.080 38.359 38.359 38.925 36.031 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 -3.256 -4.229 -2.571 -2.863 -3.747 -2.948 -4.919 -1.517 -0.563 -1.416 -2.440 -0.163 -0.561 -1.615 0.379 | 44.939 43.519 44.907 45.613 46.970 40.875 41.154 40.865 39.765 39.945 38.631 37.544 36.423 35.619 37.015 36.939 37.040 36.316 36.217 35.696 34.968 35.861 34.737 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 19.10 1.00 19.10 1.00 15.34 1.00 15.34 1.00 16.21 1.00 16.00 1.00 16.41 1.00 16.54 1.00 16.89 1.00 19.20 1.00 19.20 1.00 19.20 1.00 19.20 1.00 22.58 1.00 22.28 1.00 22.19 1.00 22.73 1.00 22.73 1.00 20.42 |
| | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16638 16640 16641 16642 16644 16645 16646 16647 16650 16651 16652 16653 16655 16656 16657 16658 | CE1 CD2 CE2 CZ OH CA CB CB CC O N CA CB CB CC CB CC CC CC CC CC CC CC CC CC | TYR TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA ALA THR THR THR THR THR THR THR PRO PRO PRO PRO PRO PRO PRO PRO PRO PR | 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 2492 2492 2492 2492 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 32.016 34.218 34.948 34.196 35.127 34.507 33.628 33.753 35.476 34.705 36.655 37.710 37.080 38.359 38.359 38.925 36.031 35.718 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 -3.256 -4.229 -2.571 -2.863 -3.747 -2.948 -4.919 -1.517 -0.563 -1.416 -2.440 -0.163 -0.163 -0.561 -1.615 0.379 1.567 | 44.939 43.519 44.907 45.613 46.990 40.875 41.154 40.687 40.865 39.765 39.945 38.631 37.544 36.423 35.619 37.015 36.939 37.040 36.316 36.217 35.696 34.968 34.737 34.752 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 19.10 1.00 19.10 1.00 15.49 1.00 15.34 1.00 16.21 1.00 16.54 1.00 16.41 1.00 16.54 1.00 16.54 1.00 16.54 1.00 16.54 1.00 17.42 1.00 19.01 1.00 16.56 1.00 19.20 1.00 17.78 1.00 20.58 1.00 22.28 1.00 22.28 1.00 22.19 1.00 22.73 1.00 22.77 1.00 20.07 |
| | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 16634 16635 16636 16637 16639 16640 16641 16642 16644 16645 16647 16646 16650 16651 16652 16653 16655 16655 | CE1 CD2 CE2 CZ CC OH CA CB CA CB CC CB CC | TYR TYR TYR TYR TYR TYR TYR TYR ALA ALA ALA ALA THR THR THR THR THR PRO PRO PRO PRO PRO PRO PRO | 2490 2490 2490 2490 2490 2490 2491 2491 2491 2491 2492 2492 2492 2492 | 35.062 33.011 33.017 34.042 34.038 33.652 34.842 32.821 33.240 32.016 34.948 34.196 35.127 34.507 33.628 33.753 35.476 34.705 36.655 37.710 37.080 38.359 38.359 38.925 36.031 | 1.572 2.795 2.855 2.244 2.326 -0.390 -0.532 -1.413 -2.806 -3.716 -3.256 -4.229 -2.571 -2.863 -3.747 -2.948 -4.919 -1.517 -0.563 -1.416 -2.440 -0.163 -0.561 -1.615 0.379 | 44.939 43.519 44.907 45.613 46.970 40.875 41.154 40.865 39.765 39.945 38.631 37.544 36.423 35.619 37.015 36.939 37.040 36.316 36.217 35.696 34.968 35.861 34.737 | 1.00 18.54 1.00 20.42 1.00 20.22 1.00 19.10 1.00 19.10 1.00 15.34 1.00 15.34 1.00 16.21 1.00 16.00 1.00 16.41 1.00 16.54 1.00 16.89 1.00 19.20 1.00 19.20 1.00 19.20 1.00 19.20 1.00 22.58 1.00 22.28 1.00 22.19 1.00 22.73 1.00 22.73 1.00 20.42 |

| ATOM | 16661 | CB | GLU | 2494 | 34.027 | -1.249 | 32.078 | 1.00 27.93 |
|------|-------|-----|-----|------|--------|--------|--------|------------|
| ATOM | 16662 | CG | GLU | 2494 | 33.193 | -0.865 | 30.862 | 1.00 35.30 |
| ATOM | 16663 | CD | GLU | 2494 | 33.127 | -1.979 | 29.825 | 1.00 39.26 |
| ATOM | 16664 | | GLU | 2494 | 32.813 | -3.129 | 30.207 | 1.00 40.58 |
| ATOM | 16665 | | GLU | 2494 | 33.381 | -1.701 | 28.629 | 1.00 41.62 |
| ATOM | 16666 | C | GLU | 2494 | 33.296 | 0.596 | 33.629 | 1.00 21.02 |
| | | | | 2494 | 32.867 | 1.674 | 33.236 | 1.00 20.30 |
| MOTA | 16667 | 0 | GLU | | | | | |
| MOTA | 16668 | N | GLN | 2495 | 32.768 | -0.043 | 34.663 | 1.00 19.92 |
| MOTA | 16669 | CA | GLN | 2495 | 31.638 | 0.536 | 35.377 | 1.00 21.90 |
| MOTA | 16670 | CB | GLN | 2495 | 31.103 | -0.446 | 36.411 | 1.00 25.01 |
| MOTA | 16671 | CG | GLN | 2495 | 30.627 | -1.747 | 35.803 | 1.00 32.47 |
| MOTA | 16672 | CD | GLN | 2495 | 29.946 | -2.626 | 36.814 | 1.00 34.62 |
| MOTA | 16673 | OE1 | GLN | 2495 | 28.836 | -2.332 | 37.259 | 1.00 37.69 |
| ATOM | 16674 | NE2 | GLN | 2495 | 30.614 | -3.707 | 37.202 | 1.00 39.43 |
| MOTA | 16675 | С | GLN | 2495 | 32.044 | 1.835 | 36.056 | 1.00 18.71 |
| ATOM | 16676 | 0 | GLN | 2495 | 31.269 | 2.788 | 36.101 | 1.00 16.24 |
| ATOM | 16677 | N | ALA | 2496 | 33.263 | 1.870 | 36.583 | 1.00 18.87 |
| ATOM | 16678 | CA | ALA | 2496 | 33.756 | 3.073 | 37.236 | 1.00 18.29 |
| ATOM | 16679 | СВ | ALA | 2496 | 35.161 | 2.842 | 37.789 | 1.00 19.37 |
| ATOM | 16680 | C | ALA | 2496 | 33.758 | 4.249 | 36.258 | 1.00 17.83 |
| ATOM | 16681 | 0 | ALA | 2496 | 33.373 | 5.355 | 36.626 | 1.00 17.54 |
| | | | | | 34.181 | 4.018 | 35.014 | 1.00 17.34 |
| MOTA | 16682 | N | PHE | 2497 | | | | |
| MOTA | 16683 | CA | PHE | 2497 | 34.215 | 5.104 | 34.033 | 1.00 16.32 |
| MOTA | 16684 | CB | PHE | 2497 | 34.777 | 4.639 | 32.680 | 1.00 15.77 |
| MOTA | 16685 | CG | PHE | 2497 | 36.109 | 3.944 | 32.763 | 1.00 16.08 |
| MOTA | 16686 | | PHE | 2497 | 37.023 | 4.262 | 33.763 | 1.00 17.05 |
| MOTA | 16687 | CD2 | PHE | 2497 | 36.453 | 2.976 | 31.822 | 1.00 19.05 |
| MOTA | 16688 | CE1 | PHE | 2497 | 38.264 | 3.626 | 33.831 | 1.00 18.78 |
| ATOM | 16689 | CE2 | PHE | 2497 | 37.686 | 2.334 | 31.876 | 1.00 18.30 |
| MOTA | 16690 | CZ | PHE | 2497 | 38.594 | 2.660 | 32.885 | 1.00 19.48 |
| ATOM | 16691 | С | PHE | 2497 | 32.817 | 5.659 | 33.796 | 1.00 16.99 |
| ATOM | 16692 | ō | PHE | 2497 | 32.616 | 6.872 | 33.761 | 1.00 15.02 |
| ATOM | 16693 | N | GLU | 2498 | 31.860 | 4.753 | 33.624 | 1.00 17.61 |
| ATOM | 16694 | CA | GLU | 2498 | 30.474 | 5.121 | 33.364 | 1.00 19.06 |
| | 16695 | CB | GLU | 2498 | 29.635 | 3.854 | 33.162 | 1.00 22.66 |
| MOTA | | | | | 28.212 | 4.090 | 32.676 | 1.00 28.82 |
| MOTA | 16696 | CG | GLU | 2498 | | | | |
| MOTA | 16697 | CD. | GLU | 2498 | 28.165 | 4.785 | 31.322 | 1.00 33.26 |
| ATOM | 16698 | | GLU | 2498 | 29.130 | 4.638 | 30.536 | 1.00 33.89 |
| MOTA | 16699 | OE2 | | 2498 | 27.156 | 5.469 | 31.038 | 1.00 35.72 |
| ATOM | 16700 | C | GLU | 2498 | 29.880 | 5.947 | 34.499 | 1.00 18.47 |
| MOTA | 16701 | О | GLU | 2498 | 29.368 | 7.049 | 34.281 | 1.00 19.38 |
| MOTA | 16702 | N | ASN | 2499 | 29.954 | 5.413 | 35.711 | 1.00 18.25 |
| ATOM | 16703 | CA | ASN | 2499 | 29.392 | 6.105 | 36.869 | 1.00 19.15 |
| MOTA | 16704 | CB | ASN | 2499 | 29.335 | 5.157 | 38.070 | 1.00 19.68 |
| MOTA | 16705 | CG | ASN | 2499 | 28.385 | 3.997 | 37.839 | 1.00 19.41 |
| MOTA | 16706 | OD1 | ASN | 2499 | 27.309 | 4.178 | 37.269 | 1.00 21.49 |
| ATOM | 16707 | | ASN | 2499 | 28.767 | 2.811 | 38.283 | 1.00 18.16 |
| ATOM | 16708 | C | ASN | 2499 | 30.125 | 7.397 | 37.225 | 1.00 19.51 |
| ATOM | 16709 | 0 | ASN | 2499 | 29.513 | 8.347 | 37.723 | 1.00 18.86 |
| ATOM | 16710 | N | ALA | 2500 | 31.429 | 7.440 | 36.965 | 1.00 20.06 |
| ATOM | 16711 | | | 2500 | 32.207 | 8.641 | 37.239 | 1.00 19.16 |
| | | CA | ALA | | | | 37.233 | |
| ATOM | 16712 | CB | ALA | 2500 | 33.694 | 8.367 | | 1.00 19.94 |
| ATOM | 16713 | Ç | ALA | 2500 | 31.748 | 9.734 | 36.284 | 1.00 19.10 |
| ATOM | 16714 | 0 | ALA | 2500 | 31.472 | 10.858 | 36.695 | 1.00 18.94 |
| ATOM | 16715 | N | ALA | 2501 | 31.652 | 9.389 | 35.004 | 1.00 17.77 |
| MOTA | 16716 | CA | ALA | 2501 | 31.229 | 10.339 | 33.991 | 1.00 16.26 |
| MOTA | 16717 | CB | ALA | 2501 | 31.220 | 9.670 | 32.608 | 1.00 16.19 |
| ATOM | 16718 | С | ALA | 2501 | 29.850 | 10.905 | 34.303 | 1.00 15.89 |
| ATOM | 16719 | 0 | ALA | 2501 | 29.592 | 12.070 | 34.028 | 1.00 18.58 |
| ATOM | 16720 | N | THR | 2502 | 28.963 | 10.081 | 34.862 | 1.00 16.35 |
| MOTA | 16721 | CA | THR | 2502 | 27.605 | 10.524 | 35.200 | 1.00 16.80 |
| ATOM | 16722 | CB | THR | 2502 | 26.731 | 9.356 | 35.721 | 1.00 18.71 |
| ATOM | 16723 | OG1 | | 2502 | 26.565 | 8.386 | 34.685 | 1.00 18.62 |
| ATOM | 16724 | CG2 | | 2502 | 25.358 | 9.859 | 36.148 | 1.00 18.69 |
| ATOM | 16725 | C | THR | 2502 | 27.629 | 11.594 | 36.281 | 1.00 16.73 |
| ATOM | 16726 | 0 | THR | 2502 | 26.919 | 12.592 | 36.204 | 1.00 16.10 |
| ATOM | 16727 | N | VAL | 2502 | 28.441 | 11.355 | 37.301 | 1.00 16.73 |
| | | | | | 28.582 | 12.280 | 38.416 | 1.00 10.73 |
| MOTA | 16728 | CA | VAL | 2503 | | | | |
| MOTA | 16729 | CB | VAL | 2503 | 29.336 | 11.588 | 39.565 | 1.00 21.79 |
| MOTA | 16730 | | VAL | 2503 | 29.985 | 12.604 | 40.454 | 1.00 26.41 |
| ATOM | 16731 | | VAL | 2503 | 28.365 | 10.712 | 40.355 | 1.00 18.83 |
| ATOM | 16732 | C | VAL | 2503 | 29.321 | 13.541 | 37.962 | 1.00 18.67 |
| MOTA | 16733 | 0 | VAL | 2503 | 29.040 | 14.649 | 38.435 | 1.00 18.94 |
| MOTA | 16734 | N | MET | 2504 | 30.260 | 13.362 | 37.037 | 1.00 18.34 |
| ATOM | 16735 | CA | MET | 2504 | 31.026 | 14.471 | 36.495 | 1.00 19.37 |
| MOTA | 16736 | CB | MET | 2504 | 32.211 | 13.958 | 35.669 | 1.00 22.55 |
| ATOM | 16737 | CG | MET | 2504 | 33.240 | 13.157 | 36.459 | 1.00 26.75 |

| ATOM | 16738 | SD | MET | 2504 | 34.195 | 14.200 | 37.555 | 1.00 33.58 |
|------------------------------|----------------------------------|------------------------|------------|----------------------|----------------------------|-------------------------|----------------------------|--|
| ATOM | 16739 | CE | MET | 2504 | 35.397 | 14.833 | 36.400 | 1.00 29.91 |
| | | | | | | | | |
| MOTA | 16740 | С | MET | 2504 | 30.138 | 15.357 | 35.623 | 1.00 19.08 |
| MOTA | 16741 | 0 | MET | 2504 | 30.170 | 16.573 | 35.755 | 1.00 16.51 |
| MOTA | 16742 | N | ARG | 2505 | 29.341 | 14.757 | 34.738 | 1.00 18.93 |
| ATOM | 16743 | CA | ARG | 2505 | 28.476 | 15.553 | 33.883 | 1.00 19.02 |
| | | | ARG | 2505 | 27.748 | 14.672 | 32.853 | 1.00 19.49 |
| MOTA | 16744 | CB | | | | | | |
| ATOM | 16745 | CG | ARG | 2505 | 28.673 | 13.917 | 31.888 | 1.00 22.49 |
| MOTA | 16746 | CD | ARG | 2505 | 27.903 | 13.299 | 30.717 | 1.00 23.75 |
| MOTA | 16747 | NE | ARG | 2505 | 28.708 | 12.314 | 29.985 | 1.00 25.72 |
| MOTA | 16748 | CZ | ARG | 2505 | 28.734 | 11.015 | 30.268 | 1.00 24.59 |
| | | | | | | | | |
| MOTA | 16749 | NH1 | ARG | 2505 | 27.997 | 10.536 | 31.261 | 1.00 22.81 |
| MOTA | 16750 | NH2 | ARG | 2505 | 29.505 | 10.197 | 29.569 | 1.00 26.75 |
| MOTA | 16751 | С | ARG | 2505 | 27.451 | 16.298 | 34.728 | 1.00 17.69 |
| ATOM | 16752 | 0 | ARG | 2505 | 26.955 | 17.351 | 34.327 | 1.00 18.42 |
| | 16753 | N | ALA | 2506 | 27.145 | 15.755 | 35.902 | 1.00 17.09 |
| ATOM | | | | | | | | |
| MOTA | 16754 | CA | ALA | 2506 | 26.164 | 16.363 | 36.800 | 1.00 18.48 |
| ATOM | 16755 | CB | ALA | 2506 | 25.652 | 15.325 | 37.797 | 1.00 17.12 |
| ATOM | 16756 | С | ALA | 2506 | 26.713 | 17.580 | 37.551 | 1.00 18.29 |
| ATOM | 16757 | 0 | ALA | 2506 | 25.957 | 18.298 | 38.208 | 1.00 18.33 |
| ATOM | 16758 | N | GLY | 2507 | 28.020 | 17.807 | 37.448 | 1.00 18.55 |
| | | | | | | | | |
| MOTA | 16759 | CA | GLY | 2507 | 28.622 | 18.958 | 38.098 | 1.00 19.92 |
| MOTA | 16760 | C | GLY | 2507 | 29.863 | 18.732 | 38.943 | 1.00 20.81 |
| MOTA | 16761 | 0 | GLY | 2507 | 30.537 | 19.694 | 39.333 | 1.00 20.95 |
| ATOM | 16762 | N | ALA | 2508 | 30.183 | 17.478 | 39.238 | 1.00 20.50 |
| ATOM | 16763 | CA | ALA | 2508 | 31.354 | 17.193 | 40.062 | 1.00 19.08 |
| | | | | | | | | |
| MOTA | 16764 | CB | ALA | 2508 | 31.328 | 15.748 | 40.526 | 1.00 18.45 |
| MOTA | 16765 | С | ALA | 2508 | 32.669 | 17.482 | 39.348 | 1.00 19.05 |
| MOTA | 16766 | 0 | ALA | 2508 | 32.776 | 17.332 | 38.134 | 1.00 18.04 |
| ATOM | 16767 | N | ASN | 2509 | 33.675 | 17.899 | 40.109 | 1.00 19.09 |
| MOTA | 16768 | CA | ASN | 2509 | 34.981 | 18.184 | 39.529 | 1.00 18.59 |
| | | | | | | | | |
| MOTA | 16769 | CB | ASN | 2509 | 35.627 | 19.405 | 40.186 | 1.00 20.73 |
| MOTA | 16770 | CG | ASN | 2509 | 34.883 | 20.679 | 39.903 | 1.00 18.72 |
| MOTA | 16771 | OD1 | ASN | 2509 | 34.720 | 21.074 | 38.748 | 1.00 17.99 |
| MOTA | 16772 | ND2 | ASN | 2509 | 34.424 | 21.338 | 40.957 | 1.00 18.40 |
| ATOM | 16773 | C | ASN | 2509 | 35.905 | 17.000 | 39.756 | 1.00 19.28 |
| | | | | | | | | |
| MOTA | 16774 | 0 | ASN | 2509 | 36.841 | 16.777 | 38.992 | 1.00 18.91 |
| MOTA | 16775 | N | MET | 2510 | 35.626 | 16.246 | 40.812 | 1.00 17.99 |
| MOTA | 16776 | CA | MET | 2510 | 36.448 | 15.115 | 41.203 | 1.00 19.45 |
| MOTA | 16777 | CB | MET | 2510 | 37.466 | 15.577 | 42.251 | 1.00 18.97 |
| MOTA | 16778 | CG | MET | 2510 | 38.433 | 14.524 | 42.759 | 1.00 23.50 |
| | | | | | | | | |
| MOTA | 16779 | SD | MET | 2510 | 39.624 | 15.270 | 43.945 | 1.00 23.85 |
| MOTA | 16780 | CE | MET | 2510 | 41.036 | 15.618 | 42.863 | 1.00 24.62 |
| ATOM | 16781 | С | MET | 2510 | 35.576 | 14.020 | 41.784 | 1.00 20.19 |
| MOTA | 16782 | 0 | MET | 2510 | 34.505 | 14.289 | 42.327 | 1.00 18.96 |
| MOTA | 16783 | N | VAL | 2511 | 36.047 | 12.783 | 41.665 | 1.00 21.32 |
| ATOM | 16784 | CA | VAL | 2511 | 35.321 | | 42.156 | 1.00 20.08 |
| | | | | | | | | |
| MOTA | 16785 | CB | VAL | 2511 | 35.189 | 10.586 | 41.023 | 1.00 23.58 |
| MOTA | 16786 | CG1 | VAL | 2511 | 34.622 | 9.304 | 41.560 | 1.00 26.75 |
| MOTA | 16787 | CG2 | VAL | 2511 | 34.316 | 11.146 | 39.908 | 1.00 23.78 |
| ATOM | 16788 | С | VAL | 2511 | 36.035 | 10.991 | 43.347 | 1.00 19.91 |
| ATOM | 16789 | ō | VAL | 2511 | 37.267 | 10.916 | 43.369 | 1.00 18.34 |
| | | | | | | | 44.340 | 1.00 17.54 |
| MOTA | 16790 | N | LYS | 2512 | 35.268 | 10.547 | | |
| MOTA | 16791 | CA | LYS | 2512 | 35.850 | 9.902 | 45.513 | 1.00 18.90 |
| ATOM | 16792 | CB | LYS | 2512 | 35.473 | 10.648 | 46.803 | 1.00 19.77 |
| ATOM | 16793 | CG | LYS | 2512 | 36.064 | 9.979 | 48.044 | 1.00 21.40 |
| ATOM | 16794 | CD | LYS | 2512 | 36.198 | 10.915 | 49.233 | 1.00 23.09 |
| ATOM | 16795 | CE | LYS | 2512 | 34.908 | 11.031 | 50.024 | 1.00 23.73 |
| | | | | | | | | |
| MOTA | 16796 | NZ | LYS | 2512 | 34.461 | 9.709 | 50.567 | 1.00 21.38 |
| MOTA | 16797 | С | LYS | 2512 | 35.407 | 8.442 | 45.620 | 1.00 19.54 |
| ATOM | 16798 | 0 | LYS | 2512 | 34.219 | 8.137 | 45.525 | 1.00 20.01 |
| MOTA | 16799 | N | ILE | 2513 | 36.370 | 7.545 | 45.817 | 1.00 17.93 |
| ATOM | 16800 | CA | ILE | 2513 | 36.085 | 6.117 | 45.923 | 1.00 17.40 |
| | | | | | | | | |
| MOTA | 16801 | CB | ILE | 2513 | 36.447 | 5.384 | 44.607 | 1.00 17.97 |
| MOTA | 16802 | CG2 | ILE | 2513 | 35.518 | 5.836 | 43.489 | 1.00 17.02 |
| MOTA | 16803 | CG1 | ILE | 2513 | 37.896 | 5.694 | 44.213 | 1.00 18.73 |
| MOTA | 16804 | CD1 | ILE | 2513 | 38.353 | 4.974 | 42.946 | 1.00 18.72 |
| ATOM | 16805 | C | ILE | 2513 | 36.849 | 5.491 | 47.084 | 1.00 18.41 |
| MOTA | | | | 2513 | 37.994 | 5.858 | 47.353 | 1.00 18.45 |
| | 16806 | . 0 | ILE | | | | | |
| MOTA | 16807 | N | GLU | 2514 | 36.204 | 4.548 | 47.765 | 1.00 18.60 |
| MOTA | 16808 | CA | GLU | 2514 | 36.776 | 3.861 | 48.922 | 1.00 18.49 |
| MOTA | 4 6000 | CB | GLU | 2514 | 35.662 | 3.542 | 49.925 | 1.00 19.81 |
| 111011 | 16809 | | | | 24 027 | 4 742 | EO 260 | |
| | | | GLU | 2514 | 34.84/ | 4./43 | 50.360 | 1.00 20.46 |
| MOTA | 16810 | CG | GLU | 2514 2514 | 34.827 33.621 | 4.743 | | |
| MOTA MOTA | 16810 16811 | CG CD | GLU | 2514 | 33.621 | 4.347 | 51.222 | 1.00 23.36 |
| MOTA MOTA MOTA | 16810 16811 16812 | CG CD OE1 | GLU GLU | 2514 2514 | 33.621 33.542 | 4.347 3.176 | 51.222 51.644 | 1.00 23.36 1.00 22.24 |
| MOTA MOTA MOTA MOTA | 16810 16811 16812 16813 | CG CD OE1 OE2 | GLU GLU | 2514 2514 2514 | 33.621 33.542 32.760 | 4.347 3.176 5.212 | 51.222 51.644 51.484 | 1.00 23.36 1.00 22.24 1.00 23.56 |
| MOTA MOTA MOTA | 16810 16811 16812 | CG CD OE1 | GLU GLU | 2514 2514 | 33.621 33.542 | 4.347 3.176 | 51.222 51.644 | 1.00 23.36 1.00 22.24 |

| MOTA | 16815 | 0 | GLU | 2514 | | 37.045 | 1.777 | 47.755 | 1.00 18.14 |
|------|-------|-----|-----|--------------|---|--------|--------|------------------|------------|
| ATOM | 16816 | N | GLY | 2515 | | 38.665 | 2.339 | 49.189 | 1.00 20.64 |
| ATOM | 16817 | CA | GLY | 2515 | | 39.389 | 1.117 | 48.896 | 1.00 20.29 |
| ATOM | 16818 | C | GLY | 2515 | | 40.890 | 1.288 | 48.808 | 1.00 19.74 |
| ATOM | 16819 | ō | GLY | 2515 | | 41.393 | 2.371 | 48.501 | 1.00 18.88 |
| ATOM | 16820 | N | GLY | 2516 | | 41.602 | 0.198 | 49.065 | 1.00 19.47 |
| ATOM | 16821 | CA | GLY | 2516 | | 43.052 | 0.224 | 49.033 | 1.00 18.59 |
| ATOM | 16822 | C | GLY | 2516 | • | 43.687 | -0.132 | 47.703 | 1.00 18.48 |
| ATOM | 16823 | o | GLY | 2516 | | 43.242 | 0.303 | 46.639 | 1.00 17.54 |
| ATOM | 16824 | N | GLU | 2517 | | 44.725 | -0.955 | 47.769 | 1.00 20.76 |
| ATOM | 16825 | CA | GLU | 2517 | | 45.467 | -1.341 | 46.580 | 1.00 23.29 |
| ATOM | 16826 | СВ | GLU | 2517 | | 46.637 | -2.242 | 46.974 | 1.00 27.23 |
| ATOM | 16827 | CG | GLU | 2517 | | 47.689 | -2.380 | 45.888 | 1.00 32.03 |
| ATOM | 16828 | CD | GLU | 2517 | | 48.937 | -3.090 | 46.367 | 1.00 36.09 |
| ATOM | 16829 | | GLU | 2517 | | 49.853 | -3.300 | 45.539 | 1.00 38.84 |
| ATOM | 16830 | | GLU | 2517 | | 49.005 | -3.435 | 47.569 | 1.00 37.39 |
| MOTA | 16831 | C | GLU | 2517 | | 44.676 | -1.992 | 45.445 | 1.00 23.15 |
| ATOM | 16832 | 0 | GLU | 2517 | | 45.079 | -1.892 | 44.286 | 1.00 22.58 |
| ATOM | 16833 | N | TRP | 2518 | | 43.560 | -2.652 | 45.749 | 1.00 22.67 |
| ATOM | 16834 | CA | TRP | 2518 | | 42.791 | -3.292 | 44.682 | 1.00 23.53 |
| ATOM | 16835 | CB | TRP | 2518 | | 41.619 | -4.120 | 45.244 | 1.00 24.36 |
| ATOM | 16836 | CG | TRP | 2518 | | 40.473 | -3.335 | 45.824 | 1.00 24.10 |
| ATOM | 16837 | | TRP | 2518 | | 39.271 | -2.943 | 45.143 | 1.00 23.30 |
| ATOM | 16838 | | TRP | 2518 | | 38.466 | -2.252 | 46.078 | 1.00 23.70 |
| ATOM | 16839 | | TRP | 2518 | | 38.797 | -3.108 | 43.837 | 1.00 22.85 |
| | 16840 | | TRP | 2518 | | 40.352 | -2.874 | 47.107 | 1.00 25.21 |
| MOTA | | | TRP | 2518 | | 39.147 | -2.226 | 47.266 | 1.00 23.21 |
| MOTA | 16841 | | | | | 37.209 | -1.726 | 45.745 | 1.00 24.45 |
| ATOM | 16842 | | TRP | 2518 2518 | | | -2.585 | 43.743 | 1.00 22.85 |
| MOTA | 16843 | | TRP | | | 37.541 | | | 1.00 20.90 |
| MOTA | 16844 | | TRP | 2518 | | 36.765 | -1.903 | 44.456 | 1.00 20.30 |
| ATOM | 16845 | C | TRP | 2518 | | 42.267 | -2.282 | 43.666 | |
| MOTA | 16846 | .0 | TRP | 2518 | | 41.875 | -2.651 | 42.560 44.042 | 1.00 24.23 |
| MOTA | 16847 | N | LEU | 2519 | | 42.283 | -1.006 | | 1.00 21.97 |
| MOTA | 16848 | CA | LEU | 2519 | | 41.804 | 0.080 | 43.184 | 1.00 19.59 |
| MOTA | 16849 | CB | LEU | 2519 | | 41.185 | 1.180 | 44.043 | 1.00 20.80 |
| MOTA | 16850 | CG | LEU | 2519 | | 39.771 | 0.921 | 44.553 | 1.00 20.95 |
| MOTA | 16851 | | LEU | 2519 | | 39.347 | 2.037 | 45.517 | 1.00 20.03 |
| MOTA | 16852 | | LEU | 2519 | | 38.824 | 0.853 | 43.358 | 1.00 19.11 |
| MOTA | 16853 | С | LEU | 2519 | | 42.855 | 0.724 | 42.292 | 1.00 20.90 |
| MOTA | 16854 | О | LEU | 2519 | | 42.525 | 1.556 | 41.444 | 1.00 20.68 |
| ATOM | 16855 | N | VAL | 2520 | | 44.117 | 0.361 | 42.483 | 1.00 19.40 |
| MOTA | 16856 | CA | VAL | 2520 | | 45.186 | 0.955 | 41.692 | 1.00 18.98 |
| ATOM | 16857 | CB | VAL | 2520 | | 46.513 | 0.172 | 41.864 | 1.00 19.23 |
| MOTA | 16858 | | VAL | 2520 | | 47.524 | 0.629 | 40.825 | 1.00 20.17 |
| | 16859 | | VAL | 2520 | | 47.073 | 0.413 | 43.262 | 1.00 21.65 |
| MOTA | 16860 | C | VAL | 2520 | | 44.870 | 1.070 | 40.206 | 1.00 18.55 |
| ATOM | 16861 | 0 | VAL | 2520 | | 44.981 | 2.149 | 39.630 | 1.00 18.33 |
| ATOM | 16862 | N | GLU | 2521 | | 44.475 | -0.037 | 39.590 | 1.00 17.61 |
| ATOM | 16863 | CA | GLU | 2521 | | 44.159 | -0.037 | 38.168 | 1.00 21.27 |
| MOTA | 16864 | CB | GLU | 2521 | | 43.770 | -1.448 | 37.729 | |
| MOTA | 16865 | CG | GLU | 2521 | | 43.404 | -1.568 | 36.261 | 1.00 31.82 |
| ATOM | 16866 | CD | GLU | 2521 | | 43.139 | -3.009 | 35.856 | |
| MOTA | 16867 | | GLU | 2521 | | 42.203 | -3.633 | 36.408 | 1.00 37.34 |
| MOTA | 16868 | | GLU | 2521 | | 43.871 | -3.520 | 34.985 | 1.00 39.34 |
| MOTA | 16869 | C. | GLU | 2521 | | 43.037 | 0.942 | 37.828 | 1.00 19.73 |
| ATOM | 16870 | Ò | GLU | 2521 | | 43.137 | 1.721 | 36.879 | 1.00 18.47 |
| MOTA | 16871 | N | THR | 2522 | | 41.967 | 0.909 | 38.611 | 1.00 18.72 |
| MOTA | 16872 | CA | THR | 2522 | | 40.834 | 1.789 | 38.360 | 1.00 17.06 |
| MOTA | 16873 | CB | THR | 2522 | | 39.696 | 1.466 | 39.341 | 1.00 17.53 |
| MOTA | 16874 | | THR | 2522 | | 39.327 | 0.087 | 39.182 | 1.00 18.32 |
| MOTA | 16875 | CG2 | | 2522 | | 38.481 | 2.339 | 39.074 | 1.00 16.11 |
| MOTA | 16876 | C | THR | 2522 | | 41.232 | 3.256 | 38.469 | 1.00 17.09 |
| MOTA | 16877 | 0 | THR | 2522 | | 40.808 | 4.089 | 37.668 | 1.00 16.74 |
| ATOM | 16878 | N | VAL | 2523 | | 42.060 | 3.580 | 39.452 | 1.00 18.90 |
| MOTA | 16879 | CA | VAL | 2523 | | 42.488 | 4.968 | 39.614 | 1.00 18.66 |
| ATOM | 16880 | СВ | VAL | 2523 | | 43.295 | 5.155 | 40.910 | 1.00 19.35 |
| MOTA | 16881 | | VAL | 2523 | | 43.779 | 6.595 | 41.011 | 1.00 20.95 |
| ATOM | 16882 | | VAL | 2523 | | 42.442 | 4.799 | 42.116 | 1.00 18.48 |
| ATOM | 16883 | С | VAL | 2523 | | 43.345 | 5.398 | 38.419 | 1.00 18.29 |
| MOTA | 16884 | 0 | VAL | 2523 | | 43.141 | 6.476 | 37.858 | 1.00 18.36 |
| MOTA | 16885 | N | GLN | 2524 | | 44.309 | 4.563 | 38.038 | 1.00 16.98 |
| ATOM | 16886 | CA | GLN | 2524 | | 45.174 | 4.894 | 36.907 | 1.00 19.97 |
| ATOM | 16887 | CB | GLN | 2524 | | 46.169 | 3.761 | 36.626 | 1.00 21.97 |
| MOTA | 16888 | CG | GLN | 2524 | | 47.125 | 3.462 | 37.769 | 1.00 28.49 |
| MOTA | 16889 | CD | GLN | 2524 | | 48.108 | 2.355 | 37.429 | 1.00 32.31 |
| MOTA | 16890 | | GLN | 2524 | | 47.711 | 1.273 | 36.998 | 1.00 33.90 |
| MOTA | 16891 | NE2 | GLN | 2524 | | 49.400 | 2.619 | 37.627 | 1.00 32.72 |

| ATOM | 16892 | С | GLN | 2524 | 44.359 | 5.153 | 35.648 | 1.00 20.47 |
|--------------|----------------|----------|------------|--------------|------------------|------------------|------------------|--------------------------|
| ATOM | 16893 | Ō | GLN | 2524 | 44.572 | 6.146 | 34.950 | 1.00 19.34 |
| ATOM | 16894 | N | MET | 2525 | 43.420 | 4.258 | 35.360 | 1.00 19.30 |
| MOTA | 16895 | CA | MET | 2525 | 42.600 | 4.385 | 34.163 | 1.00 20.94 |
| MOTA | 16896 | CB | MET | 2525 | 41.853 | 3.076 | 33.908 | 1.00 20.76 |
| MOTA | 16897 | CG | MET | 2525 | 42.796 | 1.931 | 33.555 | 1.00 22.97 |
| MOTA | 16898 | SD | MET | 2525 | 41.953 | 0.379 | 33.211 | 1.00 25.66 |
| MOTA | 16899 | CE | MET | 2525 | 41.613 | 0.585 | 31.487 | 1.00 26.72 |
| MOTA | 16900 | С | MET | 2525 | 41.638 | 5.558 | 34.213 | 1.00 21.37 |
| MOTA | 16901 | 0 | MET | 2525 | 41.439 | 6.233 | 33.208 | 1.00 21.66 |
| ATOM | 16902 | N | LEU | 2526 | 41.044 | 5.808 | 35.375 | 1.00 21.24 |
| ATOM | 16903 | CA | LEU | 2526 | 40.129 39.502 | 6.935 6.964 | 35.503 36.900 | 1.00 20.80 1.00 17.52 |
| ATOM ATOM | 16904 16905 | CB CG | LEU LEU | 2526 2526 | 38.292 | 6.075 | 37.149 | 1.00 17.32 |
| ATOM | 16906 | | LEU | 2526 | 37.996 | 6.041 | 38.641 | 1.00 15.92 |
| ATOM | 16907 | | LEU | 2526 | 37.095 | 6.606 | 36.373 | 1.00 16.60 |
| ATOM | 16908 | C | LEU | 2526 | 40.878 | 8.241 | 35.263 | 1.00 21.12 |
| ATOM | 16909 | ō | LEU | 2526 | 40.404 | 9.124 | 34.546 | 1.00 21.66 |
| ATOM | 16910 | N | THR | 2527 | 42.059 | 8.353 | 35.860 | 1.00 22.05 |
| ATOM | 16911 | CA | THR | 2527 | 42.875 | 9.555 | 35.725 | 1.00 24.14 |
| MOTA | 16912 | CB | THR | 2527 | 44.186 | 9.419 | 36.521 | 1.00 24.39 |
| MOTA | 16913 | OG1 | THR | 2527 | 43.879 | 9.270 | 37.914 | 1.00 27.58 |
| ATOM | 16914 | CG2 | THR | 2527 | 45.061 | 10.656 | 36.334 | 1.00 27.09 |
| MOTA | 16915 | С | THR | 2527 | 43.217 | 9.883 | 34.276 | 1.00 25.83 |
| MOTA | 16916 | 0 | THR | 2527 | 43.061 | 11.020 | 33.838 | 1.00 26.77 |
| MOTA | 16917 | N | GLU | 2528 | 43.679 | 8.888 | 33.529 | 1.00 27.93 |
| MOTA | 16918 | CA | GLU | 2528 | 44.042 | 9.127 | 32.138 | 1.00 29.80 |
| ATOM | 16919 | CB | GLU | 2528 | 44.815 | 7.935 | 31.578 31.350 | 1.00 31.80 1.00 32.54 |
| MOTA MOTA | 16920 16921 | CG CD | GLU GLU | 2528 2528 | 43.995 44.836 | 6.697 5.567 | 30.791 | 1.00 32.34 |
| ATOM | 16921 | OE1 | | 2528 | 45.737 | 5.857 | 29.977 | 1.00 35.69 |
| ATOM | 16923 | | GLU | 2528 | 44.599 | 4.397 | 31.157 | 1.00 33.65 |
| MOTA | 16924 | C | GLU | 2528 | 42.827 | 9.429 | 31.265 | 1.00 28.28 |
| MOTA | 16925 | ō | GLU | 2528 | 42.971 | 9.896 | 30.135 | 1.00 28.14 |
| MOTA | 16926 | N | ARG | 2529 | 41.634 | 9.174 | 31.797 | 1.00 28.80 |
| MOTA | 16927 | CA | ARG | 2529 | 40.395 | 9.431 | 31.069 | 1.00 28.26 |
| MOTA | 16928 | CB | ARG | 2529 | 39.452 | 8.230 | 31.205 | 1.00 26.83 |
| MOTA | 16929 | CG | ARG | 2529 | 39.946 | 7.014 | 30.427 | 1.00 26.61 |
| MOTA | 16930 | CD | ARG | 2529 | 39.231 | 5.732 | 30.796 | 1.00 23.98 |
| MOTA | 16931 | NE | ARG | 2529 | 39.737 | 4.615 | 30.003 | 1.00 24.06 |
| ATOM | 16932 | CZ | ARG | 2529 | 40.992 | 4.180 | 30.041 | 1.00 25.03 |
| ATOM | 16933 | | ARG | 2529 | 41.879 | 4.759 3.171 | 30.838 29.270 | 1.00 23.39 1.00 24.77 |
| ATOM | 16934 | NH2 C | ARG ARG | 2529 2529 | 41.368 39.702 | 10.713 | 31.530 | 1.00 24.77 |
| MOTA MOTA | 16935 16936 | 0 | ARG | 2529 | 38.478 | 10.713 | 31.465 | 1.00 28.70 |
| ATOM | 16937 | N | ALA | 2530 | 40.503 | 11.667 | 32.001 | 1.00 28.59 |
| ATOM | 16938 | CA | ALA | 2530 | 40.018 | 12.970 | 32.452 | 1.00 26.75 |
| ATOM | 16939 | СВ | ALA | 2530 | 39.218 | 13.637 | 31.332 | 1.00 29.24 |
| ATOM | 16940 | C | ALA | 2530 | 39.196 | 12.970 | 33.737 | 1.00 26.34 |
| ATOM | 16941 | 0 | ALA | 2530 | 38.391 | 13.876 | 33.953 | 1.00 25.02 |
| MOTA | 16942 | Ŋ | VAL | 2531 | 39.400 | 11.974 | 34.595 | 1.00 23.38 |
| MOTA | 16943 | CA | VAL | | 38.655 | 11.907 | 35.849 | 1.00 23.24 |
| MOTA | 16944 | CB | VAL | 2531 | 37.802 | 10.617 | 35.933 | 1.00 22.38 |
| ATOM | 16945 | CG1 | | 2531 | 37.001 | 10.605 | 37.222 | 1.00 24.98 |
| MOTA | 16946 | CG2 | | 2531 | 36.874 | 10.530 | 34.740 | 1.00 23.60 |
| MOTA | 16947 | C | VAL | 2531 | 39.549 | 11.968 | 37.089 | 1.00 22.08 1.00 20.71 |
| ATOM | 16948 | O N | VAL | 2531 2532 | 40.180 39.618 | 10.979 13.137 | 37.464 37.743 | 1.00 20.71 |
| MOTA MOTA | 16949 16950 | N CD | PRO PRO | 2532 | 38.951 | 14.412 | 37.439 | 1.00 23.52 |
| ATOM | 16951 | CA | PRO | 2532 | 40.450 | 13.259 | 38.944 | 1.00 22.45 |
| ATOM | 16952 | CB | PRO | 2532 | 40.414 | 14.757 | 39.238 | 1.00 22.66 |
| ATOM | 16953 | CG | PRO | 2532 | 39.070 | 15.148 | 38.756 | 1.00 25.65 |
| MOTA | 16954 | C | PRO | 2532 | 39.836 | 12.421 | 40.057 | 1.00 21.12 |
| MOTA | 16955 | 0 | PRO | 2532 | 38.623 | 12.446 | 40.255 | 1.00 21.74 |
| ATOM | 16956 | N | VAL | 2533 | 40.673 | 11.678 | 40.773 | 1.00 19.42 |
| MOTA | 16957 | CA | VAL | 2533 | 40.208 | 10.802 | 41.837 | 1.00 18.80 |
| MOTA | 16958 | CB | VAL | 2533 | 40.670 | 9.345 | 41.596 | 1.00 18.15 |
| ATOM | 16959 | | VAL | 2533 | 40.209 | 8.462 | 42.736 | 1.00 19.03 |
| MOTA | 16960 | | VAL | 2533 | 40.134 | 8.832 | 40.263 | 1.00 18.13 |
| ATOM | 16961 | С | VAL | 2533 | 40.696 | 11.181 | 43.220 | 1.00 18.90 |
| ATOM | 16962 | O | VAL | 2533 | 41.844 | 11.587 | 43.389 44.204 | 1.00 19.13 1.00 17.65 |
| ATOM | 16963 | N | CYS | 2534 2534 | 39.813 40.143 | 11.044 11.296 | 44.204 | 1.00 17.65 |
| ATOM ATOM | 16964 16965 | CA CB | CYS CYS | 2534 | 39.125 | 12.250 | 46.259 | 1.00 17.23 |
| MOTA | 16966 | SG | CYS | 2534 | 39.435 | 12.575 | 48.025 | 1.00 10.32 |
| MOTA | 16967 | C | CYS | 2534 | 40.038 | 9.922 | 46.265 | 1.00 17.85 |
| MOTA | 16968 | Ö | CYS | 2534 | 39.004 | 9.258 | 46.159 | 1.00 20.42 |

| MOTA | 16969 | N | GLY | 2535 | 41.107 | 9.481 | 46.917 | 1.00 16.91 |
|--------------|----------------|------------|------------|--------------|------------------|------------------|------------------|--------------------------|
| MOTA | 16970 | CA | GLY | 2535 | 41.084 | 8.192 | 47.580 | 1.00 17.14 |
| MOTA | 16971 | С | GLY | 2535 | 40.382 | 8.290 | 48.921 | 1.00 18.33 |
| MOTA | 16972 | 0 | GLY | 2535 | 40.041 | 9.388 | 49.362 | 1.00 19.66 |
| MOTA | 16973 | N | HIS | 2536 | 40.168 | 7.149 | 49.568 | 1.00 17.24 |
| ATOM | 16974 | CA | HIS | 2536 | 39.504 | 7.106 | 50.869 | 1.00 18.82 |
| ATOM | 16975 | CB | HIS | 2536 | 37.980 | 7.162 | 50.683 | 1.00 20.25 |
| ATOM | 16976 | CG | HIS | 2536 | 37.207 | 7.331 | 51.956 53.248 | 1.00 18.55 1.00 19.79 |
| MOTA | 16977 | CD2 ND1 | | 2536 2536 | 37.537 35.897 | 7.091 7.761 | 51.971 | 1.00 20.89 |
| ATOM ATOM | 16978 16979 | CE1 | | 2536 | 35.453 | 7.777 | 53.215 | 1.00 20.03 |
| ATOM | 16980 | NE2 | HIS | 2536 | 36.428 | 7.373 | 54.010 | 1.00 20.24 |
| ATOM | 16981 | C | HIS | 2536 | 39.922 | 5.823 | 51.575 | 1.00 18.66 |
| ATOM | 16982 | 0 | HIS | 2536 | 39.620 | 4.717 | 51.123 | 1.00 19.56 |
| ATOM | 16983 | N | LEU | 2537 | 40.639 | 5.984 | 52.680 | 1.00 18.70 |
| MOTA | 16984 | CA | LEU | 2537 | 41.127 | 4.855 | 53.455 | 1.00 17.87 |
| MOTA | 16985 | CB | LEU | 2537 | 42.650 | 4.771 | 53.338 | 1.00 19.01 |
| ATOM | 16986 | CG | LEU | 2537 | 43.229 | 4.387 | 51.973 | 1.00 16.20 |
| MOTA | 16987 | CD1 | | 2537 | 44.757 | 4.537 | 51.995 | 1.00 16.71 |
| ATOM | 16988 | CD2 | LEU | 2537 | 42.851 | 2.929 | 51.653 | 1.00 17.55 |
| MOTA | 16989 | C | LEU | 2537 | 40.737 | 4.977 | 54.926 | 1.00 19.09 |
| MOTA | 16990 | 0 | LEU | 2537 | 40.273 | 6.026 | 55.371 55.670 | 1.00 20.25 1.00 18.13 |
| MOTA | 16991 16992 | N CA | GLY GLY | 2538 2538 | 40.960 | 3.901 3.882 | 57.078 | 1.00 18.13 |
| ATOM ATOM | 16993 | CA | GLY | 2538 | 39.275 | 3.253 | 57.287 | 1.00 21.82 |
| MOTA | 16994 | 0 | GLY | 2538 | 39.013 | 2.131 | 56.843 | 1.00 22.22 |
| MOTA | 16995 | N | LEU | 2539 | 38.394 | 3.980 | 57.959 | 1.00 21.58 |
| MOTA | 16996 | CA | LEU | 2539 | 37.059 | 3.470 | 58.193 | 1.00 22.62 |
| MOTA | 16997 | CB | LEU | 2539 | 36.478 | 4.096 | 59.464 | 1.00 23.08 |
| ATOM | 16998 | CG | LEU | 2539 | 35.394 | 3.309 | 60.206 | 1.00 25.71 |
| MOTA | 16999 | CD1 | LEU | 2539 | 34.896 | 4.150 | 61.377 | 1.00 27.15 |
| MOTA | 17000 | | LEU | 2539 | 34.254 | 2.962 | 59.280 | 1.00 24.37 |
| MOTA | 17001 | С | LEU | 2539 | 36.213 | 3.830 | 56.977 | 1.00 22.01 |
| MOTA | 17002 | 0 | LEU | 2539 | 35.665 | 4.931 | 56.897 | 1.00 24.68 |
| MOTA | 17003 | N | THR | 2540 | 36.139 | 2.909 | 56.020 | 1.00 21.79 |
| ATOM | 17004 | CA | THR | 2540 | 35.350 | 3.100 | 54.801 53.599 | 1.00 23.60 1.00 22.72 |
| MOTA | 17005 17006 | CB OG1 | THR | 2540 2540 | 35.991 36.312 | 2.337 0.996 | 53.991 | 1.00 22.72 |
| ATOM ATOM | 17007 | CG2 | THR | 2540 | 37.258 | 3.035 | 53.143 | 1.00 25.28 |
| ATOM | 17007 | C | THR | 2540 | 33.934 | 2.574 | 55.072 | 1.00 23.37 |
| ATOM | 17009 | o | THR | 2540 | 33.680 | 1.371 | 54.992 | 1.00 23.82 |
| ATOM | 17010 | N | PRO | 2541 | 32.997 | 3.483 | 55.403 | 1.00 24.67 |
| MOTA | 17011 | CD | PRO | 2541 | 33.189 | 4.941 | 55.330 | 1.00 25.29 |
| MOTA | 17012 | CA | PRO | 2541 | 31.595 | 3.165 | 55.711 | 1.00 23.91 |
| MOTA | 17013 | CB | PRO | 2541 | 30.927 | 4.543 | 55.801 | 1.00 25.13 |
| MOTA | 17014 | CG | PRO | 2541 | 31.817 | 5.420 | 54.989 | 1.00 29.14 |
| MOTA | 17015 | С | PRO | 2541 | 30.866 | 2.212 | 54.777 | 1.00 22.03 |
| MOTA | 17016 | 0 | PRO | 2541 | 29.964 | 1.489 | 55.212 | 1.00 21.27 |
| MOTA | 17017 | N | GLN | 2542 | 31.241 | 2.196 | 53.504 | 1.00 21.17 |
| MOTA | 17018 | CA | GLN | 2542 | 30.593 31.081 | 1.280 | 52.562 51.126 | 1.00 20.34 |
| MOTA | 17019 17020 | CB CG | GLN GLN | 2542 2542 | 30.468 | 1.542 2.776 | 50.462 | 1.00 19.40 |
| ATOM ATOM | 17020 | CD | GLN | 2542 | 31.057 | 3.072 | 49.090 | 1.00 20.00 |
| ATOM | 17022 | OE1 | | 2542 | 31.534 | 2.172 | 48.399 | 1.00 21.78 |
| ATOM | 17023 | NE2 | GLN | 2542 | 31.014 | 4.335 | 48.686 | 1.00 18.53 |
| ATOM | 17024 | С | GLN | 2542 | 30.887 | -0.166 | 52.962 | 1.00 20.22 |
| MOTA | 17025 | 0 | GLN | 2542 | 30.106 | -1.067 | 52.659 | 1.00 21.15 |
| MOTA | 17026 | N | SER | 2543 | 32.005 | -0.381 | 53.655 | 1.00 21.08 |
| MOTA | 17027 | CA | SER | 2543 | 32.392 | -1.725 | 54.089 | 1.00 20.09 |
| MOTA | 17028 | CB | SER | 2543 | 33.903 | -1.934 | 53.925 | 1.00 22.29 |
| MOTA | 17029 | OG | SER | 2543 | 34.275 | -2.037 | 52.553 | 1.00 22.70 |
| MOTA | 17030 | С | SER | 2543 | 32.009 | -2.008 | 55.541 | 1.00 20.40 |
| MOTA | 17031 | 0 | SER | 2543 | 32.533 | -2.938 | 56.162 | 1.00 19.84 |
| ATOM | 17032 | N | VAL | 2544 | 31.084 30.644 | -1.218 -1.391 | 56.077 57.455 | 1.00 19.14 1.00 20.23 |
| ATOM ATOM | 17033 17034 | CA CB | VAL VAL | 2544 2544 | 29.416 | -0.473 | 57.774 | 1.00 20.23 |
| ATOM | 17034 | | VAL | 2544 | 28.242 | -0.473 | 56.867 | 1.00 21.04 |
| ATOM | 17036 | | VAL | 2544 | 29.031 | -0.615 | 59.235 | 1.00 24.52 |
| ATOM | 17037 | C | VAL | 2544 | 30.301 | -2.847 | 57.775 | 1.00 19.12 |
| ATOM | 17038 | ō | VAL | 2544 | 30.623 | -3.343 | 58.854 | 1.00 17.37 |
| MOTA | 17039 | N | ASN | 2545 | 29.659 | -3.533 | 56.835 | 1.00 20.26 |
| MOTA | 17040 | CA | ASN | 2545 | 29.288 | -4.923 | 57.041 | 1.00 21.25 |
| MOTA | 17041 | CB | ASN | 2545 | 28.350 | -5.383 | 55.921 | 1.00 20.97 |
| ATOM | 17042 | CG | ASN | 2545 | 27.009 | -4.683 | 55.969 | 1.00 19.71 |
| ATOM | 17043 | | ASN | 2545 | 26.215 | -4.912 | 56.881 | 1.00 19.36 |
| MOTA | 17044 | | ASN | 2545 | 26.755 | -3.806 | 54.997 | 1.00 20.75 |
| MOTA | 17045 | С | ASN | 2545 | 30.521 | -5.820 | 57.101 | 1.00 22.83 |

| MOTA | 17046 | 0 | ASN | 2545 | 30.499 | -6.877 | 57.726 | 1.00 23.72 |
|------|-------|-----|-----|------|--------|---------|--------|------------|
| ATOM | 17047 | N | ILE | 2546 | 31.594 | -5.395 | 56.443 | 1.00 22.99 |
| | | | | | | | | |
| MOTA | 17048 | CA | ILE | 2546 | 32.839 | -6.154 | 56.447 | 1.00 24.98 |
| MOTA | 17049 | CB | ILE | 2546 | 33.842 | -5.623 | 55.379 | 1.00 25.25 |
| ATOM | 17050 | CG2 | ILE | 2546 | 35.189 | -6.332 | 55.529 | 1.00 24.01 |
| | | | | | | | | |
| MOTA | 17051 | CG1 | ILE | 2546 | 33.295 | ~5.852 | 53.968 | 1.00 25.29 |
| MOTA | 17052 | CD1 | ILE | 2546 | 33.166 | -7.330. | 53.587 | 1.00 25.88 |
| ATOM | 17053 | C | ILE | 2546 | 33.485 | -6.028 | 57.827 | 1.00 26.31 |
| | | | | | | | | |
| MOTA | 17054 | 0 | ILE | 2546 | 33.852 | -7.027 | 58.445 | 1.00 25.76 |
| ATOM | 17055 | N | PHE | 2547 | 33.606 | -4.794 | 58.309 | 1.00 26.71 |
| | 17056 | CA | PHE | 2547 | 34.214 | -4.534 | 59.615 | 1.00 29.32 |
| MOTA | | | | | | | | |
| MOTA | 17057 | CB | PHE | 2547 | 34.482 | -3.033 | 59.802 | 1.00 29.87 |
| MOTA | 17058 | CG | PHE | 2547 | 35.258 | -2.401 | 58.679 | 1.00 32.32 |
| ATOM | 17059 | | PHE | 2547 | 36.474 | -2.939 | 58.258 | 1.00 33.03 |
| | | | | | | | | |
| MOTA | 17060 | CD2 | PHE | 2547 | 34.782 | -1.253 | 58.054 | 1.00 32.76 |
| MOTA | 17061 | CE1 | PHE | 2547 | 37.204 | -2.342 | 57.229 | 1.00 32.42 |
| MOTA | 17062 | CE2 | PHE | 2547 | 35.504 | -0.647 | 57.024 | 1.00 33.54 |
| | | | | | | | | |
| MOTA | 17063 | CZ | PHE | 2547 | 36.719 | -1.195 | 56.612 | 1.00 33.74 |
| ATOM | 17064 | С | PHE | 2547 | 33.325 | -5.011 | 60.756 | 1.00 30.19 |
| ATOM | 17065 | 0 | PHE | 2547 | 33.814 | -5.329 | 61.837 | 1.00 31.92 |
| | | | | | | | | |
| MOTA | 17066 | N | GLY | 2548 | 32.020 | -5.063 | 60.509 | 1.00 30.16 |
| ATOM | 17067 | CA | GLY | 2548 | 31.093 | -5.483 | 61.541 | 1.00 30.32 |
| ATOM | 17068 | С | GLY | 2548 | 30.665 | -4.284 | 62.367 | 1.00 31.76 |
| | | | | | | | | |
| MOTA | 17069 | 0 | GLY | 2548 | 30.281 | -4.412 | 63.529 | |
| ATOM | 17070 | N | GLY | 2549 | 30.741 | -3.106 | 61.756 | 1.00 32.09 |
| MOTA | 17071 | CA | GLY | 2549 | 30.361 | -1.882 | 62.438 | 1.00 31.70 |
| | | | | | | | | |
| ATOM | 17072 | С | GLY | 2549 | 31.326 | -0.764 | 62.095 | 1.00 31.81 |
| ATOM | 17073 | . 0 | GLY | 2549 | 32.223 | -0.943 | 61.273 | 1.00 30.10 |
| ATOM | 17074 | N | TYR | 2550 | 31.151 | 0.394 | 62.722 | 1.00 32.22 |
| | | | | | | | | |
| MOTA | 17075 | CA | TYR | 2550 | 32.030 | 1.525 | 62.467 | |
| MOTA | 17076 | CB | TYR | 2550 | 31.229 | 2.827 | 62.456 | 1.00 34.84 |
| ATOM | 17077 | CG | TYR | 2550 | 30.084 | 2.806 | 61.470 | 1.00 36.99 |
| | | | | 2550 | | | | 1.00 37.25 |
| ATOM | 17078 | CD1 | TYR | | 28.863 | 2.207 | 61.800 | |
| MOTA | 17079 | CE1 | TYR | 2550 | 27.821 | 2.140 | 60.875 | 1.00 38.43 |
| ATOM | 17080 | CD2 | TYR | 2550 | 30.233 | 3.339 | 60.189 | 1.00 37.03 |
| ATOM | 17081 | CE2 | TYR | 2550 | 29.201 | 3.275 | 59.255 | 1.00 37.75 |
| | | | | | | | | |
| MOTA | 17082 | CZ | TYR | 2550 | 27.999 | 2.675 | 59.600 | 1.00 38.27 |
| MOTA | 17083 | OH | TYR | 2550 | 26.986 | 2.600 | 58.671 | 1.00 36.43 |
| MOTA | 17084 | С | TYR | 2550 | 33.105 | 1.564 | 63.546 | 1.00 34.34 |
| ATOM | 17085 | ō | TYR | 2550 | 32.948 | 2.226 | 64.572 | 1.00 35.56 |
| | | | | | | | | |
| MOTA | 17086 | N | LYS | 2551 | 34.194 | 0.840 | 63.306 | 1.00 32.76 |
| MOTA | 17087 | CA | LYS | 2551 | 35.298 | 0.752 | 64.254 | 1.00 32.19 |
| ATOM | 17088 | CB | LYS | 2551 | 35.598 | -0.719 | 64.546 | 1.00 34.81 |
| ATOM | 17089 | CG | LYS | 2551 | 34.364 | -1.541 | 64.900 | 1.00 38.01 |
| | | | | | | | | |
| ATOM | 17090 | CD | LYS | 2551 | 34.699 | -3.015 | 65.008 | 1.00 40.22 |
| ATOM | 17091 | CE | LYS | 2551 | 33.462 | -3.851 | 65.283 | 1.00 41.88 |
| ATOM | 17092 | NZ | LYS | 2551 | 33.802 | -5.302 | 65.396 | 1.00 44.79 |
| | | | | | | | | |
| MOTA | 17093 | С | LYS | 2551 | 36.553 | 1.435 | 63.719 | 1.00 30.37 |
| MOTA | 17094 | 0 | LYS | 2551 | 36.786 | 1.462 | 62.513 | 1.00 30.25 |
| ATOM | 17095 | N | VAL | 2552 | 37.363 | 1.982 | 64.619 | 1.00 29.43 |
| ATOM | 17096 | CA | VAL | 2552 | 38.590 | 2.658 | 64.215 | 1.00 28.03 |
| | | | | | | | | |
| MOTA | 17097 | CB | VAL | 2552 | 39.312 | 3.274 | 65.433 | 1.00 28.51 |
| MOTA | 17098 | CG1 | VAL | 2552 | 40.619 | 3.922 | 65.001 | 1.00 26.74 |
| MOTA | 17099 | | VAL | 2552 | 38.410 | 4.304 | 66.096 | 1.00 26.18 |
| | | | | | | | | |
| MOTA | 17100 | С | VAL | 2552 | 39.512 | 1.662 | 63.518 | 1.00 27.85 |
| ATOM | 17101 | 0 | VAL | 2552 | 39.697 | 0.538 | 63.988 | 1.00 26.93 |
| MOTA | 17102 | N | GLN | 2553 | 40.085 | 2.080 | 62.395 | 1.00 27.87 |
| | | | | | | | | |
| ATOM | 17103 | CA | GLN | 2553 | 40.973 | 1.217 | 61.626 | 1.00 29.57 |
| MOTA | 17104 | CB | GLN | 2553 | 40.523 | 1.196 | 60.162 | 1.00 30.19 |
| MOTA | 17105 | CG | GLN | 2553 | 40.399 | -0.196 | 59.554 | 1.00 34.54 |
| | | | | | | | 60.292 | 1.00 34.33 |
| ATOM | 17106 | CD | GLN | 2553 | 39.402 | -1.069 | | |
| MOTA | 17107 | | GLN | 2553 | 38.286 | -0.641 | 60.594 | 1.00 35.02 |
| ATOM | 17108 | NE2 | GLN | 2553 | 39.798 | -2.303 | 60.582 | 1.00 37.14 |
| MOTA | 17109 | С | GLN | 2553 | 42.419 | 1.695 | 61.715 | 1.00 29.23 |
| | | | | | | | | |
| ATOM | 17110 | 0 | GLN | 2553 | 42.686 | 2.813 | 62.152 | 1.00 29.38 |
| MOTA | 17111 | N | GLY | 2554 | 43.346 | 0.837 | 61.303 | 1.00 30.12 |
| ATOM | 17112 | CA | GLY | 2554 | 44.752 | 1.200 | 61.328 | 1.00 31.55 |
| MOTA | 17113 | C | GLY | 2554 | 45.499 | 0.751 | 62.568 | 1.00 33.25 |
| | | | | | | | | 1.00 33.26 |
| ATOM | 17114 | 0 | GLY | 2554 | 46.730 | 0.754 | 62.590 | |
| MOTA | 17115 | N | ARG | 2555 | 44.755 | 0.371 | 63.602 | 1.00 33.75 |
| MOTA | 17116 | CA | ARG | 2555 | 45.350 | -0.088 | 64.851 | 1.00 34.75 |
| ATOM | 17117 | CB | ARG | 2555 | 44.253 | -0.548 | 65.818 | 1.00 36.93 |
| | | | | | | | | |
| MOTA | 17118 | CG | ARG | 2555 | 43.309 | 0.558 | 66.303 | 1.00 39.18 |
| MOTA | 17119 | CD | ARG | 2555 | 43.894 | 1.309 | 67.489 | 1.00 40.08 |
| MOTA | 17120 | NE | ARG | 2555 | 42.993 | 2.331 | 68.030 | 1.00 39.43 |
| ATOM | 17121 | CZ | ARG | 2555 | 41.807 | 2.081 | 68.580 | 1.00 40.99 |
| | | | | | | | | |
| ATOM | 17122 | NH1 | ARG | 2555 | 41.356 | 0.836 | 68.666 | 1.00 41.89 |
| | | | | | | | | |

| ATOM | 17123 | NH2 | ARG | 2555 | 41.075 | 3.079 | 69.058 | 1.00 38.37 |
|------|-------|-----|-----|------|--------|--------|--------|------------|
| ATOM | 17124 | С | ARG | 2555 | 46.310 | -1.242 | 64.581 | 1.00 34.23 |
| | | | ARG | 2555 | 45.958 | -2.208 | 63.903 | 1.00 33.15 |
| ATOM | 17125 | 0 | | | | | | 1.00 34.60 |
| MOTA | 17126 | N | GLY | 2556 | 47.523 | -1.140 | 65.114 | |
| MOTA | 17127 | CA | GLY | 2556 | 48.503 | -2.194 | 64.912 | 1.00 35.58 |
| MOTA | 17128 | C | GLY | 2556 | 49.469 | -1.893 | 63.784 | 1.00 35.76 |
| MOTA | 17129 | 0 | GLY | 2556 | 49.157 | -1.128 | 62.872 | 1.00 35.13 |
| ATOM | 17130 | N | ASP | 2557 | 50.647 | -2.505 | 63.839 | 1.00 36.48 |
| ATOM | 17131 | CA | ASP | 2557 | 51.663 | -2.282 | 62.819 | 1.00 36.98 |
| | | | | | 52.984 | -2.932 | 63.231 | 1.00 37.65 |
| MOTA | 17132 | CB | ASP | 2557 | | | | |
| ATOM | 17133 | CG | ASP | 2557 | 53.604 | -2.265 | 64.437 | 1.00 38.08 |
| MOTA | 17134 | OD1 | | 2557 | 53.271 | -1.088 | 64.697 | 1.00 38.16 |
| MOTA | 17135 | OD2 | ASP | 2557 | 54.434 | -2.909 | 65.115 | 1.00 38.66 |
| MOTA | 17136 | C | ASP | 2557 | 51.266 | -2.776 | 61.439 | 1.00 36.71 |
| ATOM | 17137 | 0 | ASP | 2557 | 51.405 | -2.049 | 60.457 | 1.00 38.15 |
| ATOM | 17138 | N | GLU | 2558 | 50.777 | -4.009 | 61.358 | 1.00 36.83 |
| ATOM | 17139 | CA | GLU | 2558 | 50.381 | -4.573 | 60.074 | 1.00 37.15 |
| | | | | | 49.895 | -6.012 | 60.242 | 1.00 40.41 |
| ATOM | 17140 | CB | GLU | 2558 | | | | |
| MOTA | 17141 | CG | GLU | 2558 | 49.768 | -6.763 | 58.928 | 1.00 44.93 |
| MOTA | 17142 | CD | GLU | 2558 | 48.831 | -7.946 | 59.018 | 1.00 47.28 |
| ATOM | 17143 | OE1 | GLU | 2558 | 49.026 | -8.794 | 59.916 | 1.00 48.79 |
| MOTA | 17144 | OE2 | GLU | 2558 | 47.899 | -8.027 | 58.187 | 1.00 48.79 |
| ATOM | 17145 | С | GLU | 2558 | 49.270 | -3.740 | 59.450 | 1.00 36.06 |
| MOTA | 17146 | ō | GLU | 2558 | 49.344 | -3.363 | 58.280 | 1.00 34.74 |
| | | | | | 48.239 | -3.456 | 60.240 | 1.00 33.89 |
| MOTA | 17147 | N | ALA | 2559 | | | | 1.00 33.89 |
| MOTA | 17148 | CA | ALA | 2559 | 47.114 | -2.665 | 59.763 | |
| MOTA | 17149 | CB | ALA | 2559 | 46.037 | -2.571 | 60.846 | 1.00 32.43 |
| MOTA | 17150 | С | ALA | 2559 | 47.590 | -1.274 | 59.366 | 1.00 30.42 |
| MOTA | 17151 | 0 | ALA | 2559 | 47.180 | -0.739 | 58.338 | 1.00 30.62 |
| ATOM | 17152 | N | GLY | 2560 | 48.460 | -0.694 | 60.188 | 1.00 28.46 |
| ATOM | 17153 | CA | GLY | 2560 | 48.978 | 0.630 | 59.898 | 1.00 26.73 |
| ATOM | 17154 | C | GLY | 2560 | 49.817 | 0.672 | 58.633 | 1.00 25.98 |
| | 17155 | ō | GLY | 2560 | 49.664 | 1.574 | 57.811 | 1.00 25.52 |
| ATOM | | | | | | | | 1.00 25.32 |
| ATOM | 17156 | N | ASP | 2561 | 50.703 | -0.305 | 58.465 | |
| ATOM | 17157 | CA | ASP | 2561 | 51.558 | -0.339 | 57.285 | 1.00 24.81 |
| MOTA | 17158 | CB | ASP | 2561 | 52.603 | -1.451 | 57.401 | 1.00 26.12 |
| ATOM | 17159 | CG | ASP | 2561 | 53.606 | -1.197 | 58.507 | 1.00 26.29 |
| MOTA | 17160 | OD1 | ASP | 2561 | 53.951 | -0.020 | 58.744 | 1.00 27.90 |
| ATOM | 17161 | | ASP | 2561 | 54.064 | -2.178 | 59.127 | 1.00 29.88 |
| ATOM | 17162 | C | ASP | 2561 | 50.731 | -0.545 | 56.022 | 1.00 24.94 |
| | 17163 | | ASP | 2561 | 51.032 | 0:020 | 54.967 | 1.00 25.26 |
| ATOM | | 0 | | | | | 56.127 | 1.00 25.61 |
| ATOM | 17164 | N | GLN | 2562 | 49.681 | -1.351 | | |
| MOTA | 17165 | CA | GLN | 2562 | 48.829 | -1.612 | 54.975 | 1.00 24.70 |
| ATOM | 17166 | CB | GLN | 2562 | 47.763 | -2.651 | 55.324 | 1.00 27.82 |
| ATOM | 17167 | CG | GLN | 2562 | 46.939 | -3.080 | 54.123 | 1.00 28.73 |
| MOTA | 17168 | CD | GLN | 2562 | 47.781 | -3.794 | 53.087 | 1.00 29.94 |
| ATOM | 17169 | OE1 | GLN | 2562 | 48.326 | -4.865 | 53.356 | 1.00 31.90 |
| ATOM | 17170 | NE2 | GLN | 2562 | 47.900 | -3.204 | 51.898 | 1.00 29.29 |
| ATOM | 17171 | C | GLN | 2562 | 48.157 | -0.327 | 54.504 | 1.00 24.50 |
| | | | | | | -0.059 | | 1.00 23.09 |
| ATOM | 17172 | 0 | GLN | 2562 | 48.084 | | 53.303 | |
| ATOM | 17173 | N | LEU | 2563 | 47.658 | 0.468 | 55.448 | 1.00 25.26 |
| ATOM | 17174 | CA | LEU | 2563 | | 1.728 | | 1.00 24.24 |
| ATOM | 17175 | CB | LEU | 2563 | 46.331 | 2.353 | 56.333 | 1.00 24.36 |
| ATOM | 17176 | CG | LEU | 2563 | 45.074 | 1.675 | 56.882 | 1.00 26.38 |
| ATOM | 17177 | | LEU | 2563 | 44.544 | 2.465 | 58.070 | 1.00 27.10 |
| ATOM | 17178 | CD2 | LEU | 2563 | 44.018 | 1.599 | 55.797 | 1.00 27.72 |
| ATOM | 17179 | C | LEU | 2563 | 48.006 | 2.707 | 54.528 | 1.00 24.78 |
| | 17180 | 0 | LEU | 2563 | 47.694 | 3.476 | 53.619 | 1.00 22.15 |
| ATOM | | | | | | | | 1.00 24.45 |
| ATOM | 17181 | N | LEU | 2564 | 49.220 | 2.682 | 55.067 | |
| MOTA | 17182 | CA | LEU | 2564 | 50.264 | 3.580 | 54.590 | 1.00 23.89 |
| MOTA | 17183 | CB | LEU | 2564 | 51.495 | 3.480 | 55.491 | 1.00 25.26 |
| MOTA | 17184 | CG | LEU | 2564 | 52.282 | 4.773 | 55.744 | 1.00 27.78 |
| MOTA | 17185 | CD1 | ĿEU | 2564 | 53.598 | 4.405 | 56.410 | 1.00 29.55 |
| MOTA | 17186 | | LEU | 2564 | 52.535 | 5.535 | 54.457 | 1.00 27.60 |
| ATOM | 17187 | C | LEU | 2564 | 50.638 | 3.173 | 53.169 | 1.00 21.75 |
| ATOM | 17188 | o | LEU | 2564 | 50.738 | 4.013 | 52.277 | 1.00 22.25 |
| ATOM | | N | | 2565 | 50.730 | 1.875 | 52.968 | 1.00 21.52 |
| | 17189 | | SER | | | | | |
| ATOM | 17190 | CA | SER | 2565 | 51.205 | 1.361 | 51.658 | 1.00 23.48 |
| MOTA | 17191 | CB | SER | 2565 | 51.473 | -0.142 | 51.745 | 1.00 26.47 |
| MOTA | 17192 | OG | SER | 2565 | 51.998 | -0.634 | 50.523 | 1.00 34.86 |
| MOTA | 17193 | С | SER | 2565 | 50.107 | 1.645 | 50.632 | 1.00 22.74 |
| MOTA | 17194 | 0 | SER | 2565 | 50.390 | 1.989 | 49.481 | 1.00 21.74 |
| ATOM | 17195 | N | ASP | 2566 | 48.853 | 1.500 | 51.054 | 1.00 19.93 |
| ATOM | 17196 | CA | ASP | 2566 | 47.718 | 1.753 | 50.168 | 1.00 18.63 |
| ATOM | 17197 | CB | ASP | 2566 | 46.399 | 1.335 | 50.836 | 1.00 19.80 |
| ATOM | | CG | | | 46.206 | -0.174 | 50.867 | 1.00 21.76 |
| | 17198 | | ASP | 2566 | | | | |
| MOTA | 17199 | ODI | ASP | 2566 | 46.935 | -0.883 | 50.146 | 1.00 24.30 |
| | | | | | | | | |

| ATOM | 17200 | OD2 | ASP | 2566 | | 45.313 | -0.655 | 51.605 | 1.00 | 20.99 |
|------|-------|-----|------------|--------------|------|--------|--------|--------|------|-------|
| ATOM | 17201 | С | ASP | 2566 | | 47.647 | 3.226 | 49.785 | 1.00 | 18.77 |
| ATOM | 17202 | 0 | ASP | 2566 | | 47.329 | 3.560 | 48.650 | 1.00 | 19.96 |
| ATOM | 17203 | N | ALA | 2567 | | 47.945 | 4.109 | 50.732 | 1.00 | 17.84 |
| ATOM | 17204 | CA | ALA | 2567 | | 47.904 | 5.536 | 50.451 | 1.00 | |
| ATOM | 17205 | СВ | ALA | 2567 | | 48.135 | 6.341 | 51.731 | 1.00 | 18.06 |
| ATOM | 17206 | C | ALA | 2567 | | 48.964 | 5.894 | 49.412 | 1.00 | |
| | | | | 2567 | | 48.705 | 6.675 | 48.504 | 1.00 | 15.81 |
| MOTA | 17207 | 0 | ALA | | | | 5.338 | 49.560 | 1.00 | |
| ATOM | 17208 | N | LEU | 2568 | | 50.162 | | | | |
| MOTA | 17209 | CA | LEU | 2568 | | 51.232 | 5.615 | 48.613 | 1.00 | 18.69 |
| MOTA | 17210 | CB | LEU | 2568 | - | 52.563 | 5.047 | 49.127 | 1.00 | |
| MOTA | 17211 | CG | LEU | 2568 | | 53.121 | 5.741 | 50.379 | 1.00 | |
| MOTA | 17212 | | LEU | 2568 | | 54.332 | 4.997 | 50.913 | | 25.07 |
| ATOM | 17213 | CD2 | LEU | 2568 | | 53.484 | 7.182 | 50.031 | | 24.13 |
| MOTA | 17214 | С | LEU | 2568 | | 50.887 | 5.011 | 47.249 | 1.00 | 18.91 |
| ATOM | 17215 | 0 | LEU | 2568 | | 51.158 | 5.611 | 46.214 | 1.00 | |
| ATOM | 17216 | N | ALA | 2569 | | 50.268 | 3.835 | 47.254 | 1.00 | 19.41 |
| MOTA | 17217 | CA | ALA | 2569 | | 49.892 | 3.155 | 46.015 | 1.00 | 20.41 |
| MOTA | 17218 | CB | ALA | 2569 | | 49.395 | 1.738 | 46.317 | 1.00 | 19.39 |
| ATOM | 17219 | С | ALA | 2569 | | 48.820 | 3.929 | 45.257 | 1.00 | 20.57 |
| MOTA | 17220 | 0 | ALA | 2569 | | 48.834 | 3.982 | 44.024 | 1.00 | 18.66 |
| ATOM | 17221 | N | LEU | 2570 | | 47.875 | 4.506 | 45.996 | 1.00 | 21.33 |
| ATOM | 17222 | CA | LEU | 2570 | | 46.810 | 5.295 | 45.385 | 1.00 | 20.35 |
| ATOM | 17223 | СВ | LEU | 2570 | | 45.718 | 5.630 | 46.412 | 1.00 | |
| ATOM | 17224 | CG | LEU | 2570 | | 44.822 | 4.476 | 46.878 | 1.00 | |
| ATOM | 17225 | | LEU | 2570 | | 43.854 | 4.960 | 47.959 | 1.00 | |
| | 17226 | | LEU | 2570 | | 44.056 | 3.926 | 45.682 | 1.00 | |
| ATOM | | | | | | 47.401 | 6.582 | 44.824 | 1.00 | |
| MOTA | 17227 | C. | LEU | 2570 | | | | 43.754 | 1.00 | 16.60 |
| MOTA | 17228 | 0 | LEU | 2570 | | 46.999 | 7.049 | 45.547 | | |
| MOTA | 17229 | N | GLU | 2571 | | 48.356 | 7.163 | | 1.00 | 19.59 |
| MOTA | 17230 | CA | GLU | 2571 | | 48.990 | 8.389 | 45.076 | 1.00 | |
| MOTA | 17231 | CB | GLU | 2571 | | 49.965 | 8.937 | 46.127 | 1.00 | 19.80 |
| MOTA | 17232 | CG | GLU | 2571 | | 50.705 | 10.184 | 45.662 | 1.00 | |
| MOTA | 17233 | CD | GLU | 2571 | | 51.688 | 10.684 | 46.706 | 1.00 | |
| ATOM | 17234 | OE1 | GLU | 2571 | | 52.470 | 9.854 | 47.213 | 1.00 | |
| MOTA | 17235 | OE2 | GLU | 2571 | | 51.677 | 11.891 | 47.003 | 1.00 | |
| ATOM | 17236 | С | GLU | 2571 | | 49.748 | 8.124 | 43.779 | 1.00 | 19.41 |
| ATOM | 17237 | 0 | GLU | 2571 | | 49.658 | 8.904 | 42.833 | 1.00 | 20.18 |
| MOTA | 17238 | N | ALA | 2572 | | 50.491 | 7.020 | 43.745 | 1.00 | 20.49 |
| ATOM | 17239 | CA | ALA | 2572 | | 51.266 | 6.660 | 42.564 | 1.00 | 21.39 |
| ATOM | 17240 | СВ | ALA | 2572 | | 52.137 | 5.453 | 42.859 | 1.00 | 23.82 |
| ATOM | 17241 | С | ALA | 2572 | | 50.347 | 6.363 | 41.388 | 1.00 | 22.09 |
| MOTA | 17242 | 0 | ALA | 2572 | | 50.718 | 6.555 | 40.228 | 1.00 | 20.31 |
| ATOM | 17243 | N | ALA | 2573 | | 49.142 | 5.903 | 41.702 | 1.00 | 22.04 |
| ATOM | 17244 | CA | ALA | 2573 | .* . | 48.152 | 5.564 | 40.689 | 1.00 | 21.67 |
| ATOM | 17245 | СВ | ALA | 2573 | | 47.038 | 4.725 | 41.313 | 1.00 | 20.41 |
| ATOM | 17246 | c | ALA | 2573 | | 47.569 | 6.807 | 40.029 | 1.00 | |
| ATOM | 17247 | Õ | ALA | 2573 | | 47.084 | 6.746 | 38.900 | 1.00 | |
| ATOM | 17248 | N | GLY | 2574 | | 47.615 | 7.934 | 40.733 | 1.00 | 19.07 |
| ATOM | 17249 | CA | GLY | 2574 | | 47.089 | 9.163 | 40.168 | | 17.50 |
| ATOM | 17250 | C | GLY | 2574 | | 46.141 | 9.944 | 41.060 | | 17.16 |
| ATOM | 17251 | 0 | GLY | 2574 | | 45.716 | 11.041 | 40.701 | | 17.95 |
| | | | ALA | 2575 | | 45.796 | 9.390 | 42.217 | 1.00 | 17.09 |
| MOTA | 17252 | N | ALA | 2575 | | 44.904 | 10.083 | 43.137 | 1.00 | 19.39 |
| MOTA | 17253 | CA | | | | 44.694 | 9.246 | 44.388 | 1.00 | 17.57 |
| MOTA | 17254 | CB | ALA ALA | 2575 2575 | | 45.516 | 11.444 | 43.498 | 1.00 | 20.74 |
| ATOM | 17255 | C | | 2575 | | 46.687 | 11.526 | 43.496 | | 22.35 |
| ATOM | 17256 | 0 | ALA | | | | | | 1.00 | 20.06 |
| MOTA | 17257 | N | GLN | 2576 | | 44.731 | 12.510 | 43.375 | | |
| ATOM | 17258 | CA | GLN | 2576 | | 45.226 | 13.848 | 43.684 | 1.00 | |
| ATOM | 17259 | CB | GLN | 2576 | | 44.733 | 14.836 | 42.628 | | 24.45 |
| ATOM | 17260 | CG | GLN | 2576 | | 45.226 | 14.509 | 41.223 | | 29.02 |
| ATOM | 17261 | CD | GLN | 2576 | | 44.551 | 15.337 | 40.149 | | 31.24 |
| MOTA | 17262 | | GLN | 2576 | | 44.686 | 16.559 | 40.109 | | 36.20 |
| MOTA | 17263 | | GLN | 2576 | | 43.811 | 14.671 | 39.271 | 1.00 | 32.65 |
| MOTA | 17264 | С | GLN | 2576 | | 44.822 | 14.316 | 45.082 | | 21.51 |
| MOTA | 17265 | 0 | GLN | 2576 | | 45.260 | 15.371 | 45.549 | 1.00 | 19.45 |
| MOTA | 17266 | N | LEU | 2577 | | 43.991 | 13.519 | | | 20.67 |
| MOTA | 17267 | CA | LEU | 2577 | | 43.517 | 13.817 | 47.093 | 1.00 | 21.57 |
| MOTA | 17268 | CB | LEU | 2577 | | 42.207 | 14.609 | 47.032 | | 25.05 |
| MOTA | 17269 | CG | LEU | 2577 | | 42.283 | 16.133 | 47.063 | 1.00 | 26.27 |
| MOTA | 17270 | | LEU | 2577 | | 40.924 | 16.728 | 46.738 | 1.00 | 27.14 |
| ATOM | 17271 | | LEU | 2577 | | 42.751 | 16.576 | 48.449 | 1.00 | 27.72 |
| ATOM | 17272 | С | LEU | 2577 | | 43.280 | 12.515 | 47.850 | 1.00 | 21.36 |
| ATOM | 17273 | ō | LEU | 2577 | | 43.059 | 11.472 | 47.239 | | 22.18 |
| ATOM | 17274 | N | LEU | 2578 | | 43.327 | 12.571 | 49.178 | 1.00 | 19.22 |
| ATOM | 17275 | CA | LEU | 2578 | | 43.085 | 11.383 | 49.991 | 1.00 | 19.03 |
| ATOM | 17276 | СВ | LEU | 2578 | | 44.403 | 10.691 | 50.389 | 1.00 | 19.80 |
| | - | | | | | | | | | |

| MOTA | 17277 | CG | LEU | 2578 | 44.235 | 9.475 | 51.320 | 1.00 20.24 |
|--------------|----------------|----------|------------|--------------|------------------|-----------------|------------------|--------------------------|
| ATOM | 17278 | | LEU | 2578 | 43.537 | 8.346 | 50.556 | 1.00 21.15 |
| ATOM | 17279 | | LEU | 2578 | 45.587 | 8.989 | 51.840 | 1.00 20.62 |
| ATOM | 17280 | C | LEU | 2578 | 42.321 | 11.722 | 51.261 | 1.00 20.13 |
| ATOM | 17281 | ō | LEU | 2578 | 42.636 | 12.694 | 51.949 | 1.00 20.75 |
| ATOM | 17282 | N | VAL | 2579 | 41.303 | 10.924 | 51.560 | 1.00 19.83 |
| MOTA | 17283 | | VAL | 2579 | 40.529 | 11.105 | 52.779 | 1.00 18.16 |
| ATOM | 17284 | CB. | VAL | 2579 | 39.000 | 11.083 | 52.508 | 1.00 17.51 |
| MOTA | 17285 | | VAL | 2579 | 38.230 | 10.860 | 53.822 | 1.00 16.02 |
| | 17286 | | VAL | 2579 | 38.569 | 12.401 | 51.890 | 1.00 17.32 |
| ATOM | 17287 | C | VAL | 2579 | 40.884 | 9.962 | 53.720 | 1.00 17.52 |
| MOTA | 17288 | 0 | VAL | 2579 | 40.874 | 8.793 | 53.720 | 1.00 19.81 |
| MOTA | 17289 | N | LEU | 2580 | 41.232 | 10.316 | 54.956 | 1.00 19.69 |
| MOTA | 17290 | CA | LEU | 2580 | 41.576 | 9.350 | 55.997 | 1.00 20.23 |
| MOTA | 17291 | CB | LEU | 2580 | 42.912 | 9.684 | 56.656 | 1.00 20.23 |
| ATOM | | CG | LEU | 2580 | 44.174 | 9.119 | 56.045 | 1.00 24.93 |
| ATOM | 17292 17293 | | LEU | 2580 | 45.332 | 9.429 | 56.983 | 1.00 22.17 |
| MOTA | 17293 | | LEU | 2580 | 44.027 | 7.607 | 55.848 | 1.00 22.17 |
| MOTA | 17294 | CDZ | LEU | 2580 | 40.510 | 9.440 | 57.063 | 1.00 22.55 |
| MOTA | 17296 | 0 | LEU | 2580 | 40.321 | 10.502 | 57.648 | 1.00 10.32 |
| MOTA | 17297 | N | GLU | 2581 | 39.840 | 8.327 | 57.330 | 1.00 20.20 |
| MOTA | 17298 | CA | GLU | 2581 | 38.759 | 8.310 | 58.308 | 1.00 19.88 |
| MOTA | 17299 | CB | GLU | 2581 | 37.452 | 7.906 | 57.611 | 1.00 20.26 |
| MOTA MOTA | 17300 | CG | GLU | 2581 | 36.289 | 7.660 | 58.564 | 1.00 22.54 |
| ATOM | 17300 | CD | GLU | 2581 | 34.945 | 7.737 | 57.869 | 1.00 24.53 |
| ATOM | 17301 | | GLU | 2581 | 34.920 | 7.787 | 56.622 | 1.00 21.82 |
| ATOM | 17302 | | GLU | 2581 | 33.912 | 7.748 | 58.572 | 1.00 26.36 |
| | | | GLU | 2581 | 38.974 | 7.416 | 59.519 | 1.00 20.50 |
| MOTA | 17304 | Ċ Ö | | 2581 | 39.317 | 6.247 | 59.388 | 1.00 17.00 |
| MOTA | 17305 17306 | N | GLU CYS | 2582 | 38.779 | 7.988 | 60.701 | 1.00 10.30 |
| MOTA | 17300 | CA | CYS | 2582 | 38.896 | 7.263 | 61.955 | 1.00 19.88 |
| MOTA | | | CYS | 2582 | 37.605 | 6.489 | 62.218 | 1.00 19.88 |
| MOTA | 17308 | CB SG | | 2582 | 36.197 | 7.601 | 62.460 | 1.00 24.19 |
| MOTA | 17309 17310 | C | CYS CYS | 2582 | 40.091 | 6.340 | 62.067 | 1.00 19.95 |
| ATOM ATOM | 17311 | 0 | CYS | 2582 | 39.963 | 5.118 | 62.120 | 1.00 21.49 |
| ATOM | 17311 | N | VAL | 2583 | 41.261 | 6.954 | 62.127 | 1.00 21.05 |
| ATOM | 17312 | CA | VAL | 2583 | 42.506 | 6.226 | 62.241 | 1.00 23.03 |
| ATOM | 17314 | CB | VAL | 2583 | 43.317 | 6.351 | 60.924 | 1.00 23.48 |
| ATOM | 17315 | CG1 | | 2583 | 43.590 | 7.812 | 60.617 | 1.00 23.25 |
| ATOM | 17316 | | VAL | 2583 | 44.609 | 5.593 | 61.029 | 1.00 25.06 |
| ATOM | 17317 | C | VAL | 2583 | 43.277 | 6.871 | 63.385 | 1.00 23.22 |
| ATOM | 17318 | Ō | VAL | 2583 | 43.094 | 8.053 | 63.675 | 1.00 22.61 |
| ATOM | 17319 | N | PRO | 2584 | 44.132 | 6.099 | 64.067 | 1.00 24.47 |
| MOTA | 17320 | CD | PRO | 2584 | 44.412 | 4.662 | 63.956 | 1.00 23.45 |
| MOTA | 17321 | CA | PRO | 2584 - | 44.891 | 6.701 | 65.163 | 1.00 24.14 |
| ATOM | 17322 | CB | PRO | 2584 | 45.745 | 5.538 | 65.680 | 1.00 25.70 |
| ATOM | 17323 | CG | PRO | 2584 | 45.792 | 4.581 | 64.518 | 1.00 28.17 |
| ATOM | 17324 | C | PRO | 2584 | 45.708 | 7.873 | 64.635 | 1.00 24.60 |
| ATOM | 17325 | 0 | PRO | 2584 | 46.285 | 7.804 | 63.545 | 1.00 23.19 |
| MOTA | 17326 | N | VAL | 2585 | 45.727 | 8.958 | 65.400 | 1.00 23.51 |
| MOTA | 17327 | CA- | VAL | 2585 | 46.444 | 10.172 | 65.025 | 1.00 23.75 |
| ATOM | 17328 | CB | VAL | 2585 | 46.511 | 11.158 | | 1.00 24.99 |
| MOTA | 17329 | CG1 | VAL | 2585 | 47.098 | 12.491 | 65.758 | 1.00 23.50 |
| MOTA | 17330 | CG2 | VAL | 2585 | 45.124 | 11.363 | 66.790 | 1.00 25.53 |
| MOTA | 17331 | С | VAL | 2585 | 47.865 | 9.895 | 64.549 | 1.00 25.46 |
| MOTA | 17332 | 0 | VAL | 2585 | 48.317 | 10.477 | 63.563 | 1.00 24.79 |
| MOTA | 17333 | N | GLU | 2586 | 48.563 | 9.002 | 65.245 | 1.00 26.45 |
| MOTA | 17334 | CA | GLU | 2586 | 49.939 | 8.683 | 64.879 | 1.00 28.54 |
| ATOM | 17335 | CB | GLU | 2586 | 50.559 | 7.688 | 65.873 | 1.00 30.14 |
| MOTA | 17336 | CG | GLU | 2586 | 49.580 | 6.852 | 66.695 | 1.00 35.51 |
| MOTA | 17337 | CD | GLU | 2586 | 48.843 | 7.665 | 67.757 | 1.00 37.22 |
| MOTA | 17338 | | GLU | 2586 | 49.464 | 8.566 | 68.363 | 1.00 38.20 |
| ATOM | 17339 | | GLU | 2586 | 47.649 | 7.388 | 67.992 | 1.00 39.25 |
| MOTA | 17340 | С | GLU | 2586 | 50.064 | 8.150 | 63.456 | 1.00 28.46 |
| ATOM | 17341 | 0 | GLU | 2586 | 51.045 | 8.425 | 62.769 | 1.00 27.67 |
| ATOM | 17342 | N | LEU | 2587 | 49.065 | 7.394 | 63.017 | 1.00 27.65 |
| ATOM | 17343 | CA | LEU | 2587 | 49.077 | 6.834 | 61.674 | 1.00 26.73 |
| ATOM | 17344 | CB | LEU | 2587 | 48.026 | 5.731 | 61.554 | 1.00 28.21 |
| MOTA | 17345 | CG | LEU | 2587 | 48.378 | 4.497 | 60.721 | 1.00 30.72 |
| MOTA | 17346 | | LEU | 2587 | 47.099 | 3.720 | 60.454 | 1.00 29.14 |
| ATOM | 17347 | | LEU | 2587 | 49.043 | 4.886 | 59.409 | 1.00 30.86 |
| ATOM | 17348 | C | LEU | 2587 | 48.785 | 7.937 | 60.654 | 1.00 26.34 |
| ATOM | 17349 | O N | LEU | 2587 | 49.398 | 7.987 | 59.583 | 1.00 24.48 |
| MOTA | 17350 | N | ALA | 2588 | 47.848 | 8.820 | 60.994 | 1.00 24.00 1.00 23.70 |
| ATOM | 17351 | CA | ALA | 2588 | 47.484 | 9.922 10.737 | 60.111 60.712 | 1.00 23.70 |
| ATOM ATOM | 17352 17353 | CB C | ALA ALA | 2588 2588 | 46.331 48.691 | 10.737 | 59.887 | 1.00 23.08 |
| ATOM | 1,,,,, | C | THA | 2,00 | 40.031 | 10.013 | 33.007 | 1.00 24.14 |

| ATOM | 17354 | 0 | ALA | 2588 | 48.839 | 11.415 | 58.822 | 1.00 22.54 |
|------|-------|-----|-----|------|------------------|--------|--------|--------------------------|
| ATOM | 17355 | N | LYS | 2589 | 49.548 | 10.904 | 60.901 | 1.00 24.22 |
| ATOM | 17356 | CA | LYS | 2589 | 50,760 | 11.709 | 60.816 | 1.00 25.74 |
| ATOM | 17357 | СВ | LYS | 2589 | 51.471 | 11.751 | 62.172 | 1.00 27.20 |
| ATOM | 17358 | CG | LYS | 2589 | 50.586 | 12.130 | 63.345 | 1.00 32.13 |
| ATOM | 17359 | CD | LYS | 2589 | 51.399 | 12.323 | 64.625 | 1.00 36.29 |
| ATOM | 17360 | CE | LYS | 2589 | 50.510 | 12.760 | 65.784 | 1.00 35.55 |
| ATOM | 17361 | NZ | LYS | 2589 | 51.296 | 13.309 | 66.917 | 1.00 39.50 |
| ATOM | 17362 | C | LYS | 2589 | 51.694 | 11.086 | 59.781 | 1.00 23.37 |
| ATOM | 17363 | ō | LYS | 2589 | 52.171 | 11.768 | 58.881 | 1.00 26.48 |
| ATOM | 17364 | N | ARG | 2590 | 51.934 | 9.785 | 59.915 | 1.00 23.58 |
| ATOM | 17365 | CA | ARG | 2590 | 52.813 | 9.062 | 59.005 | 1.00 22.93 |
| ATOM | 17366 | СВ | ARG | 2590 | 52.882 | 7.575 | 59.374 | 1.00 25.56 |
| ATOM | 17367 | CG | ARG | 2590 | 52.959 | 7.280 | 60.863 | 1.00 27.56 |
| ATOM | 17368 | CD | ARG | 2590 | 53.951 | 6.177 | 61.187 | 1.00 28.90 |
| ATOM | 17369 | NE | ARG | 2590 | 53.876 | 4.999 | 60.319 | 1.00 28.63 |
| ATOM | 17370 | CZ | ARG | 2590 | 53.110 | 3.933 | 60.536 | 1.00 30.48 |
| | 17371 | NH1 | | 2590 | 52.322 | 3.872 | 61.601 | 1.00 30.99 |
| ATOM | | NH2 | | 2590 | 53.159 | 2.903 | 59.701 | 1.00 30.22 |
| ATOM | 17372 | | | | | 9.183 | 57.556 | 1.00 22.50 |
| MOTA | 17373 | C | ARG | 2590 | 52.346 | 9.366 | 56.641 | 1.00 22.30 |
| MOTA | 17374 | 0 | ARG | 2590 | 53.152 | | 57.342 | 1.00 21.17 |
| MOTA | 17375 | N | ILE | 2591 | 51.040 | 9.073 | | |
| ATOM | 17376 | CA | ILE | 2591 | 50.493 | 9.150 | 55.993 | 1.00 19.61 |
| ATOM | 17377 | CB | ILE | 2591 | 49.023 | 8.673 | 55.980 | 1.00 20.34 1.00 21.46 |
| MOTA | 17378 | CG2 | ILE | 2591 | 48.418 | 8.871 | 54.600 | |
| ATOM | 17379 | CG1 | ILE | 2591 | 48.971 | 7.206 | 56.395 | 1.00 20.56 |
| MOTA | 17380 | CD1 | ILE | 2591 | 47.585 | 6.658 | 56.588 | 1.00 25.52 |
| MOTA | 17381 | С | ILE | 2591 | 50.591 | 10.552 | 55.410 | 1.00 20.03 |
| MOTA | 17382 | 0 | ILE | 2591 | 51.005 | 10.732 | 54.261 | 1.00 19.07 |
| MOTA | 17383 | N | THR | 2592 | 50.225 | 11.549 | 56.207 | 1.00 20.25 |
| MOTA | 17384 | CA | THR | 2592 | 50.276 | 12.928 | 55.749 | 1.00 22.08 |
| MOTA | 17385 | CB | THR | 2592 | 49.743 | 13.894 | 56.826 | 1.00 21.69 |
| MOTA | 17386 | OG1 | THR | 2592 | 48.358 | 13.615 | 57.070 | 1.00 22.71 |
| MOTA | 17387 | CG2 | THR | 2592 | 49.889 | 15.343 | 56.368 | 1.00 22.53 |
| MOTA | 17388 | С | THR | 2592 | 51.693 | 13.346 | 55.376 | 1.00 23.76 |
| MOTA | 17389 | 0 | THR | 2592 | 51.896 | 14.092 | 54.417 | 1.00 24.12 |
| ATOM | 17390 | N | GLU | 2593 | 52.676 | 12.871 | 56.129 | 1.00 25.91 |
| ATOM | 17391 | CA | GLU | 2593 | 54.059 | 13.227 | 55.834 | 1.00 27.67 |
| MOTA | 17392 | CB | GLU | 2593 | 54.936 | 13.023 | 57.071 | 1.00 29.33 |
| MOTA | 17393 | CG | GLU | 2593 | 54.427 | 13.761 | 58.299 | 1.00 33.19 |
| MOTA | 17394 | CD | GLU | 2593 | 55.367 | 13.650 | 59.486 | 1.00 36.93 |
| MOTA | 17395 | OE1 | GLU | 2593 | 55.815 | 12.520 | 59.792 | 1.00 38.76 |
| ATOM | 17396 | OE2 | GLU | 2593 | 55.649° | 14.689 | 60.121 | 1.00 38.10 |
| ATOM | 17397 | С | GLU | 2593 | 54.600 | 12.407 | 54.664 | 1.00 26.14 |
| ATOM | 17398 | 0 | GLU | 2593 | 55.381 | 12.911 | 53.855 | 1.00 26.29 |
| ATOM | 17399 | N | ALA | 2594 | 54.172 | 11.153 | 54.565 | 1.00 24.55 |
| ATOM | 17400 | CA | ALA | 2594 | 54.626 | 10.281 | 53.489 | 1.00 24.61 |
| ATOM | 17401 | СВ | ALA | 2594 | 54.252 | 8.833 | 53.801 | 1.00 24.77 |
| ATOM | 17402 | Ċ | ALA | 2594 | 54.088 | 10.679 | 52.115 | 1.00 24.72 |
| ATOM | 17403 | 0 | ALA | 2594 | 54.781 | 10.519 | 51.106 | 1.00 24.92 |
| ATOM | 17404 | N | LEU | 2595 | 52.862 | 11.198 | 52.069 | 1.00 23.86 |
| ATOM | 17405 | CA | LEU | 2595 | 52.259 | 11.602 | 50.796 | 1.00 23.39 |
| ATOM | 17406 | CB | LEU | 2595 | 50.739 | 11.377 | 50.818 | 1.00 23.16 |
| ATOM | 17407 | CG | LEU | 2595 | 50.211 | 9.935 | 50.851 | 1.00 25.00 |
| ATOM | 17408 | | LEU | 2595 | 48.681 | 9.954 | 50.756 | 1.00 24.60 |
| ATOM | 17409 | CD2 | LEU | 2595 | 50.781 | 9.145 | 49.698 | 1.00 27.49 |
| ATOM | 17410 | C | LEU | 2595 | 52.526 | 13.050 | 50.410 | 1.00 22.38 |
| ATOM | 17411 | 0 | LEU | 2595 | 52.590 | 13.934 | 51.260 | 1.00 22.82 |
| ATOM | 17412 | N | ALA | 2596 | 52.673 | 13.280 | 49.112 | 1.00 21.91 |
| ATOM | 17413 | CA | ALA | 2596 | 52.907 | 14.618 | 48.580 | 1.00 20.98 |
| ATOM | 17414 | CB | ALA | 2596 | 53.676 | 14.532 | 47.259 | 1.00 21.84 |
| ATOM | 17415 | c | ALA | 2596 | 51.551 | 15.284 | 48.358 | 1.00 21.83 |
| ATOM | 17416 | ŏ | ALA | 2596 | 51.402 | 16.500 | 48.522 | 1.00 19.07 |
| ATOM | 17417 | N | ILE | 2597 | 50.563 | 14.477 | 47.972 | 1.00 22.36 |
| ATOM | 17417 | CA | ILE | 2597 | 49.206 | 14.975 | 47.744 | 1.00 22.38 |
| ATOM | 17419 | CB | ILE | 2597 | 48.329 | 13.917 | 47.038 | 1.00 20.84 |
| ATOM | 17419 | CG2 | ILE | 2597 | 48.874 | 13.629 | 45.652 | 1.00 21.38 |
| | | CG2 | ILE | 2597 | 48.274 | 12.642 | 47.887 | 1.00 20.61 |
| ATOM | 17421 | | | | 47.252 | 11.612 | 47.410 | 1.00 20.81 |
| ATOM | 17422 | CD1 | | 2597 | 48.556 | 15.315 | 49.084 | 1.00 22.88 |
| ATOM | 17423 | С | ILE | 2597 | 48.889 | 14.724 | 50.109 | 1.00 23.26 |
| ATOM | 17424 | 0 | ILE | 2597 | 47.618 | 16.276 | 49.091 | 1.00 24.06 |
| ATOM | 17425 | N | PRO | 2598 | 47.190 | 17.134 | 47.973 | 1.00 24.28 |
| ATOM | 17426 | CD | PRO | 2598 | | 16.657 | 50.339 | 1.00 24.78 |
| MOTA | 17427 | CA | PRO | 2598 | 46.951 46.158 | 17.908 | 49.946 | 1.00 24.43 |
| MOTA | 17428 | CB | PRO | 2598 | 46.158 45.908 | 17.716 | 49.940 | 1.00 24.29 |
| ATOM | 17429 | CG | PRO | 2598 | 46.079 | 15.553 | 50.935 | 1.00 27.18 |
| MOTA | 17430 | С | PRO | 2598 | 40.079 | 10.000 | 50.555 | 1.00 43.03 |

| ATOM | 17431 | 0 | PRO | 2598 | 45.401 | 14.813 | 50.218 | 1.00 23.16 |
|--------------|----------------|-----------|-----|------|------------------|------------------|------------------|--------------------------|
| | | N | VAL | 2599 | 46.126 | 15.440 | 52.257 | 1.00 22.78 |
| MOTA | 17432 | | | 2599 | 45.360 | 14.441 | 52.237 | 1.00 22.78 |
| MOTA | 17433 | CA | VAL | | | 13.580 | 53.873 | 1.00 22.48 |
| MOTA | 17434 | CB | VAL | 2599 | 46.286 | | | |
| MOTA | 17435 | CG1 | VAL | 2599 | 45.475 | 12.535 | 54.623 | 1.00 22.67 1.00 22.46 |
| MOTA | 17436 | CG2 | VAL | 2599 | 47.350 | 12.915 | 53.013 | |
| MOTA | 17437 | C | VAL | 2599 | 44.311 | 15.133 | 53.857 | 1.00 23.71 |
| MOTA | 17438 | 0 | VAL | 2599 | 44.638 | 15.979 | 54.692 | 1.00 22.13 |
| MOTA | 17439 | N | ILE | 2600 | 43.048 | 14.779 | 53.642 | 1.00 21.85 |
| ATOM | 17440 | CA | ILE | 2600 | 41.944 | 15.360 | 54.397 | 1.00 20.33 |
| MOTA | 17441 | CB | ILE | 2600 | 40.774 | 15.719 | 53.459 | 1.00 19.87 |
| MOTA | 17442 | CG2 | ILE | 2600 | 39.599 | 16.283 | 54.269 | 1.00 20.69 |
| MOTA | 17443 | CG1 | ILE | 2600 | 41.265 | 16.720 | 52.409 | 1.00 22.41 |
| MOTA | 17444 | CD1 | ILE | 2600 | 40.294 | 16.981 | 51.262 | 1.00 23.07 |
| MOTA | 17445 | С | ILE | 2600 | 41.492 | 14.343 | 55.429 | 1.00 19.49 |
| ATOM | 17446 | 0 | ILE | 2600 | 41.199 | 13.199 | 55.094 | 1.00 18.22 |
| ATOM | 17447 | N | GLY | 2601 | 41.442 | 14.754 | 56.690 | 1.00 19.36 |
| ATOM | 17448 | CA | GLY | 2601 | 41.053 | 13.813 | 57.715 | 1.00 18.13 |
| ATOM | 17449 | С | GLY | 2601 | 39.700 | 14.052 | 58.342 | 1.00 18.77 |
| ATOM | 17450 | ō | GLY | 2601 | 39.154 | 15.155 | 58.303 | 1.00 18.02 |
| ATOM | 17451 | N | ILE | 2602 | 39.155 | 12.976 | 58.892 | 1.00 18.53 |
| MOTA | 17452 | CA | ILE | 2602 | 37.892 | 12.998 | 59.600 | 1.00 19.83 |
| ATOM | 17453 | CB | ILE | 2602 | 36.684 | 12.679 | 58.671 | 1.00 21.77 |
| ATOM | 17454 | CG2 | ILE | 2602 | 36.964 | 11.449 | 57.822 | 1.00 21.95 |
| | | CG1 | ILE | 2602 | 35.424 | 12.479 | 59.518 | 1.00 24.57 |
| MOTA | 17455 | | | | 35.090 | | 60.403 | 1.00 24.37 |
| ATOM | 17456 | CD1 | ILE | 2602 | | 13.650 | | |
| MOTA | 17457 | С | ILE | 2602 | 38.059 | 11.919 | 60.658 | 1.00 19.03 |
| MOTA | 17458 | 0 | ILE | 2602 | 38.075 | 10.724 | 60.354 | 1.00 20.33 |
| MOTA | 17459 | N | GLY | 2603 | 38.217 | 12.352 | 61.901 | 1.00 16.91 |
| ATOM | 17460 | CA | GLY | 2603 | 38.431 | 11.411 | 62.980 | 1.00 18.24 |
| MOTA | 17461 | С | GLY | 2603 | 39.864 | 10.914 | 62.930 | 1.00 18.71 |
| MOTA | 17462 | 0 | GLY | 2603 | 40.169 | 9.825 | 63.410 | 1.00 19.69 |
| MOTA | 17463 | N | ALA | 2604 | 40.743 | 11.717 | 62.335 | 1.00 20.83 |
| ATOM | 17464 | CA | ALA | 2604 | 42.160 | 11.363 | 62.210 | 1.00 22.46 |
| MOTA | 17465 | CB | ALA | 2604 | 42.534 | 11.229 | 60.735 | 1.00 21.76 |
| MOTA | 17466 | С | ALA | 2604 | 43.076 | 12.382 | 62.885 | 1.00 23.51 |
| MOTA | 17467 | 0 | ALA | 2604 | 44.292 | 12.370 | 62.671 | 1.00 23.26 |
| MOTA | 17468 | N | GLY | 2605 | 42.492 | 13.268 | 63.689 | 1.00 22.78 |
| MOTA | 17469 | CA | GLY | 2605 | 43.285 | 14.273 | 64.381 | 1.00 24.37 |
| ATOM | 17470 | С | GLY | 2605 | 43.540 | 15.523 | 63.560 | 1.00 23.63 |
| MOTA | 17471 | 0 | GLY | 2605 | 43.042 | 15.650 | 62.444 | 1.00 23.74 |
| MOTA | 17472 | N | ASN | 2606 | 44.322 | 16.453 | 64.102 | 1.00 22.37 |
| ATOM | 17473 | CA | ASN | 2606 | 44.610 | 17.696 | 63.391 | 1.00 22.84 |
| ATOM | 17474 | CB | ASN | 2606 | 44.614 | 18.884 | 64.368 | 1.00 24.03 |
| ATOM | 17475 | CG | ASN | 2606 | 45.751 | 18.816 | 65.384 | 1.00 27.25 |
| ATOM | 17476 | | ASN | 2606 | 45.935 | 19.737 | 66.182 | 1.00 30.24 |
| ATOM | 17477 | ND2 | ASN | 2606 | 46.513 | 17.729 | 65.360 | 1.00 21.63 |
| ATOM | 17478 | C | ASN | 2606 | 45.935 | 17.649 | 62.644 | 1.00 22.00 |
| ATOM | 17479 | ō | ASN | 2606 | 46.428 | 18.680 | 62.185 | 1.00 22.27 |
| ATOM | 17480 | N | VAL | 2607 | 46.491 | 16.450 | 62.501 | 1.00 21.97 |
| MOTA | 17481 | CA | VAL | 2607 | 47.782 | 16.264 | 61.835 | 1.00 23.06 |
| | | | | 2607 | | 14.975 | 62.343 | 1.00 25.16 |
| ATOM | 17482 17483 | CB CC1 | VAL | 2607 | 48.473 49.896 | 14.903 | 61.813 | 1.00 30.68 |
| MOTA MOTA | 17484 | CG2 | | 2607 | 48.478 | 14.951 | 63.863 | 1.00 28.00 |
| ATOM | | | | 2607 | 47.698 | 16.210 | 60.308 | 1.00 22.15 |
| | 17485 | С | VAL | | | 16.350 | 59.614 | 1.00 19.36 |
| MOTA | 17486 | 0 | VAL | 2607 | 48.708 | | | 1.00 19.30 |
| ATOM | 17487 | N | THR | 2608 | 46.489 | 16.010 | 59.791 | |
| ATOM | 17488 | CA | THR | 2608 | 46.273 | 15.945 | 58.354 | 1.00 18.55 |
| MOTA | 17489 | CB | THR | 2608 | 44.931 | 15.247 | 58.040 | 1.00 17.48 |
| MOTA | 17490 | OG1 | THR | 2608 | 43.864 | 15.942 | 58.698 | 1.00 17.94 |
| ATOM | 17491 | CG2 | THR | 2608 | 44.958 | 13.815 | 58.538 | 1.00 16.25 |
| MOTA | 17492 | С | THR | 2608 | 46.288 | 17.340 | 57.736 | 1.00 18.46 |
| MOTA | 17493 | 0 | THR | 2608 | 46.208 | 18.344 | 58.444 | 1.00 18.52 |
| ATOM | 17494 | N | ASP | 2609 | 46.392 | 17.392 | 56.414 | 1.00 18.90 |
| ATOM | 17495 | CA | ASP | 2609 | 46.438 | 18.653 | 55.685 | 1.00 19.61 |
| ATOM | 17496 | CB | ASP | 2609 | 46.858 | 18.384 | 54.238 | 1.00 20.80 |
| MOTA | 17497 | CG | ASP | 2609 | 48.209 | 17.698 | 54.143 | 1.00 22.85 |
| MOTA | 17498 | | ASP | 2609 | 49.214 | 18.315 | 54.550 | 1.00 25.80 |
| MOTA | 17499 | OD2 | ASP | 2609 | 48.269 | 16.544 | 53.662 | 1.00 25.46 |
| MOTA | 17500 | C | ASP | 2609 | 45.101 | 19.380 | 55.711 | 1.00 19.79 |
| MOTA | 17501 | 0 | ASP | 2609 | 45.051 | 20.607 | 55.693 | 1.00 18.76 |
| ATOM | 17502 | N | GLY | 2610 | 44.014 | 18.620 | 55.754 | 1.00 19.79 |
| ATOM | 17502 | CA | GLY | 2610 | 42.703 | 19.239 | 55.771 | 1.00 17.70 |
| | 17503 | | | | | | | |
| MOTA | 17503 | C | GLY | 2610 | 41.726 | 18.492 | 56.646 | 1.00 14.64 |
| MOTA MOTA | | | | | 41.726 42.051 | 18.492 17.457 | 56.646 57.224 | 1.00 14.64 1.00 17.46 |
| | 17504 | С | GLY | 2610 | | | | |

| ATOM | 17508 | CB | GLN | 2611 | 39.268 | 19.190 | 58.853 | 1.00 19.92 |
|--------------|----------------|------------|------------|--------------|------------------|------------------|------------------|--------------------------|
| ATOM | 17509 | CG | GLN | 2611 | 40.465 | 19.210 | 59.799 | 1.00 20.42 |
| ATOM | 17510 | CD | GLN | 2611 | 40.848 | 17.829 | 60.291 | 1.00 22.00 |
| MOTA | 17511 | | GLN | 2611 | 39.984 | 17.015 | 60.627 | 1.00 24.29 |
| MOTA | 17512 | NE2 | GLN | 2611 | 42.148 | 17.561 | 60.354 | 1.00 19.83 |
| MOTA | 17513 | C | GLN | 2611 | 38.164 | 18.341 | 56.800 | 1.00 17.01 |
| ATOM | 17514 | 0 | GLN | 2611 | 37.911 37.327 | 19.151 17.379 | 55.905 57.168 | 1.00 17.06 1.00 20.01 |
| ATOM | 17515 17516 | N CA | ILE ILE | 2612 2612 | 36.013 | 17.239 | 56.557 | 1.00 20.01 |
| ATOM ATOM | 17517 | CB | ILE | 2612 | 36.047 | 16.279 | 55.336 | 1.00 21.95 |
| ATOM | 17518 | CG2 | ILE | 2612 | 36.253 | 14.835 | 55.791 | 1.00 17.51 |
| ATOM | 17519 | CG1 | ILE | 2612 | 34.743 | 16.421 | 54.542 | 1.00 21.60 |
| MOTA | 17520 | CD1 | ILE | 2612 | 34.855 | 15.977 | 53.097 | 1.00 22.16 |
| MOTA | 17521 | С | ILE | 2612 | 35.043 | 16.724 | 57.611 | 1.00 23.20 |
| MOTA | 17522 | 0 | ILE | 2612 | 35.435 | 16.034 | 58.559 | 1.00 23.34 |
| MOTA | 17523 | N | LEU | 2613 | 33.774 | 17.072 | 57.458 | 1.00 25.17 |
| ATOM | 17524 17525 | CA CB | LEU | 2613 2613 | 32.774 32.932 | 16.644 17.476 | 58.416 59.686 | 1.00 27.65 1.00 31.09 |
| ATOM ATOM | 17526 | CG | LEU | 2613 | 32.465 | 16.923 | 61.030 | 1.00 34.00 |
| ATOM | 17527 | | LEU | 2613 | 32.834 | 17.930 | 62.111 | 1.00 34.54 |
| ATOM | 17528 | | LEU | 2613 | 30.962 | 16.673 | 61.020 | 1.00 35.29 |
| ATOM | 17529 | С | LEU | 2613 | 31.382 | 16.842 | 57.821 | 1.00 27.54 |
| MOTA | 17530 | 0 | LEU | 2613 | 31.168 | 17.767 | 57.044 | 1.00 26.77 |
| MOTA | 17531 | N | VAL | 2614 | 30.450 | 15.961 | 58.173 | 1.00 27.38 |
| MOTA | 17532 | CA | VAL | 2614 | 29.087 | 16.073 | 57.678 | 1.00 27.05 |
| ATOM | 17533 | CB CC1 | VAL | 2614 2614 | 28.210 26.793 | 14.890 15.037 | 58.141 57.597 | 1.00 28.19 1.00 28.81 |
| MOTA MOTA | 17534 17535 | CG1 CG2 | | 2614 | 28.825 | 13.577 | 57.671 | 1.00 28.09 |
| ATOM | 17536 | C | VAL | 2614 | 28.523 | 17.375 | 58.238 | 1.00 25.84 |
| ATOM | 17537 | ō | VAL | 2614 | 28.502 | 17.590 | 59.449 | 1.00 26.11 |
| ATOM | 17538 | N | MET | 2615 | 28.085 | 18.251 | 57.344 | 1.00 24.55 |
| MOTA | 17539 | CA | MET | 2615 | 27.541 | 19.532 | 57.753 | 1.00 22.58 |
| MOTA | 17540 | CB | MET | 2615 | 26.987 | 20.274 | 56.546 | 1.00 20.69 |
| ATOM | 17541 | CG | MET | 2615 | 25.813 | 19.564 | 55.890 | 1.00 18.65 |
| ATOM | 17542 | SD | MET | 2615 | 24.658 | 20.775 | 55.265 56.690 | 1.00 19.02 1.00 18.27 |
| ATOM ATOM | 17543 17544 | CE C | MET MET | 2615 2615 | 23.584 26.440 | 20.962 19.393 | 58.806 | 1.00 18.27 |
| ATOM | 17545 | 0 | MET | 2615 | 26.255 | 20.281 | 59.632 | 1.00 22.04 |
| ATOM | 17546 | N | HIS | 2616 | 25.701 | 18.288 | 58.776 | 1.00 21.47 |
| ATOM | 17547 | CA | HIS | 2616 | 24.627 | 18.100 | 59.737 | 1.00 21.54 |
| ATOM | 17548 | CB | HIS | 2616 | 23.741 | 16.930 | 59.314 | 1.00 21.41 |
| MOTA | 17549 | CG | HIS | 2616 | 23.013 | 17.181 | 58.030 | 1.00 18.70 |
| ATOM | 17550 | | HIS | 2616 | 23.417 | 17.071 | 56.743 | 1.00 16.47 |
| MOTA | 17551 | | HIS | 2616 2616 | 21.736 21.385 | 17.697 17.895 | 57.987 56.729 | 1.00 20.75 1.00 18.61 |
| ATOM ATOM | 17552 17553 | | HIS HIS | 2616 | 22.388 | 17.524 | 55.955 | 1.00 20.61 |
| MOTA | 17554 | C | HIS | 2616 | 25.122 | 17.916 | 61.161 | 1.00 23.40 |
| ATOM | 17555 | o | HIS | 2616 | 24.420 | 18.266 | 62.113 | 1.00 21.84 |
| ATOM | 17556 | N | ASP | 2617 | 26.328 | 17.379 | 61.322 | 1.00 24.60 |
| ATOM | 17557 | CA | ASP | 2617 | 26.880 | 17.188 | 62.664 | 1.00 28.05 |
| MOTA | 17558 | CB | ASP | 2617 | 27.918 | 16.060 | 62.677 | 1.00 29.84 |
| ATOM | 17559 | CG OD1 | ASP | 2617 | 27.311 | 14.703 | 62.396 | 1.00 32.71 |
| ATOM ATOM | 17560 17561 | | ASP ASP | 2617 2617 | 26.339 27.818 | 14.322 14.012 | 63.088 61.487 | 1.00 30.70 1.00 34.71 |
| ATOM | 17562 | C | ASP | 2617 | 27.535 | 18.473 | 63.153 | 1.00 28.63 |
| ATOM | 17563 | ō | ASP | 2617 | 27.681 | 18.679 | 64.356 | 1.00 30.14 |
| ATOM | 17564 | N | ALA | 2618 | 27.928 | 19.333 | 62.217 | 1.00 29.76 |
| MOTA | 17565 | CA | ALA | 2618 | 28.577 | 20.593 | 62.561 | 1.00 31.50 |
| MOTA | 17566 | CB | ALA | 2618 | 29.311 | 21.152 | 61.339 | 1.00 30.82 |
| ATOM | 17567 | C | ALA | 2618 | 27.606 | 21.635 | 63.116 | 1.00 32.49 |
| ATOM ATOM | 17568 17569 | N O | ALA PHE | 2618 2619 | 28.029 26.308 | 22.630 21.411 | 63.707 62.931 | 1.00 33.61 1.00 33.51 |
| ATOM | 17570 | CA | PHE | 2619 | 25.311 | 22.350 | 63.436 | 1.00 33.26 |
| ATOM | 17571 | CB | PHE | 2619 | 24.524 | 22.962 | 62.280 | 1.00 35.56 |
| ATOM | 17572 | CG | PHE | 2619 | 25.394 | 23.485 | 61.174 | 1.00 37.64 |
| MOTA | 17573 | | PHE | 2619 | 26.457 | 24.336 | 61.452 | 1.00 39.02 |
| ATOM | 17574 | | PHE | 2619 | 25.156 | 23.119 | | 1.00 38.68 |
| ATOM | 17575 | | PHE | 2619 | 27.277 | 24.814 | 60.432 | 1.00 39.78 |
| ATOM | 17576 | | PHE | 2619 | 25.969 27.030 | 23.591 24.439 | 58.821 59.114 | 1.00 39.59 1.00 40.73 |
| ATOM ATOM | 17577 17578 | CZ C | PHE PHE | 2619 2619 | 24.359 | 24.439 | 64.423 | 1.00 40.73 |
| MOTA | 17579 | 0 | PHE | 2619 | 23.247 | 22.173 | 64.642 | 1.00 32.07 |
| ATOM | 17580 | N | GLY | 2620 | 24.806 | 20.596 | 65.023 | 1.00 33.38 |
| ATOM | 17581 | CA | GLY | 2620 | 23.989 | 19.889 | 65.996 | 1.00 32.34 |
| ATOM | 17582 | C | GLY | 2620 | 22.618 | 19.483 | 65.490 | 1.00 32.02 |
| ATOM | 17583 | 0 | GLY | 2620 | 21.715 | 19.214 | 66.283 | 1.00 32.91 |
| MOTA | 17584 | N | ILE | 2621 | 22.454 | 19.435 | 64.172 | 1.00 30.10 |

| | ATOM | 17585 | CA | ILE | 2621 | 21.176 | 19.046 | 63.589 | 1.00 29.00 |
|---|------|----------------|------|-------|------|--------|--------|--------|------------|
| | ATOM | 17586 | CB | ILE | 2621 | 21.170 | 19.248 | 62.057 | 1.00 26.35 |
| | ATOM | 17587 | | ILE | 2621 | 19.867 | 18.713 | 61.464 | 1.00 25.62 |
| | | 17588 | | ILE | 2621 | 21.332 | 20.730 | 61.729 | 1.00 24.08 |
| | ATOM | | | | | 21.695 | 21.009 | 60.295 | 1.00 24.54 |
| | MOTA | 17589 | | ILE | 2621 | | | | |
| | ATOM | 17590 | C | ILE | 2621 | 20.900 | 17.581 | 63.895 | 1.00 30.31 |
| | MOTA | 17591 | 0 | ILE | 2621 | 19.780 | 17.209 | 64.224 | 1.00 29.60 |
| | MOTA | 17592 | N | THR | 2622 | 21.936 | 16.756 | 63.799 | 1.00 32.59 |
| | MOTA | 17593 | CA | THR | 2622 | 21.794 | 15.329 | 64.053 | 1.00 35.67 |
| | ATOM | 17594 | CB | THR | 2622 | 23.035 | 14.556 | 63.560 | 1.00 35.42 |
| | MOTA | 17595 | OG1 | THR | 2622 | 24.141 | 14.813 | 64.434 | 1.00 36.19 |
| | ATOM | 17596 | CG2 | THR | 2622 | 23.407 | 15.005 | 62.158 | 1.00 31.84 |
| | ATOM | 17597 | С | THR | 2622 | 21.581 | 15.037 | 65.535 | 1.00 38.18 |
| | ATOM | 17598 | ō | THR | 2622 | 22.311 | 15.549 | 66.383 | 1.00 38.40 |
| | ATOM | 17599 | N | GLY | 2623 | 20.571 | 14.220 | 65.827 | 1.00 41.10 |
| | ATOM | 17600 | CA | GLY | 2623 | 20.252 | 13.844 | 67.194 | 1.00 46.07 |
| | | 17601 | C | GLY | 2623 | 20.921 | 14.664 | 68.279 | 1.00 49.46 |
| | ATOM | | | | | 20.755 | 15.884 | 68.342 | 1.00 50.21 |
| | ATOM | 17602 | 0 | GLY | 2623 | | | | |
| | MOTA | 17603 | N | GLY | 2624 | 21.685 | 13.992 | 69.135 | 1.00 51.80 |
| | MOTA | 17604 | CA | GLY | 2624 | 22.370 | 14.681 | 70.213 | 1.00 53.86 |
| | MOTA | 17605 | С | GLY | 2624 | 23.726 | 14.086 | 70.538 | 1.00 55.07 |
| | MOTA | 17606 | 0 | GLY | 2624 | 24.670 | 14.811 | 70.856 | 1.00 56.17 |
| | ATOM | 17607 | N | HIS | 2625 | 23.829 | 12.763 | 70.461 | 1.00 55.75 |
| | MOTA | 17608 | CA | HIS | 2625 | 25.088 | 12.087 | 70.754 | 1.00 56.39 |
| | ATOM | 17609 | CB | HIS | 2625 | 24.817 | 10.702 | 71.352 | 1.00 58.60 |
| | ATOM | 17610 | CG . | HIS - | 2625 | 24.122 | 10.744 | 72.678 | 1.00 61.61 |
| | ATOM | 17611 | | HIS | 2625 | 22.939 | 10.223 | 73.083 | 1.00 62.23 |
| , | ATOM | 17612 | | HIS | 2625 | 24.651 | 11.389 | 73.776 | |
| | ATOM | 17613 | | HIS | 2625 | 23.825 | 11.264 | 74.799 | 1.00 62.69 |
| | ATOM | 17614 | | HIS | 2625 | 22.778 | 10.561 | 74.406 | 1.00 63.05 |
| | | | C | HIS | 2625 | 25.957 | 11.959 | 69.504 | 1.00 55.11 |
| | MOTA | 17615 | | | | | | | 1.00 55.29 |
| | ATOM | 17616 | 0 | HIS | 2625 | 26.250 | 10.852 | 69.053 | |
| | MOTA | 17617 | N | ILE | 2626 | 26.368 | | 68.953 | 1.00 53.22 |
| | ATOM | 17618 | CA | ILE | 2626 | 27.207 | 13.123 | 67.756 | 1.00 50.84 |
| | MOTA | 17619 | CB | ILE | 2626 | 27.596 | 14.566 | 67.365 | 1.00 51.18 |
| | MOTA | 17620 | CG2 | ILE | 2626 | 26.352 | 15.369 | 67.024 | 1.00 52.29 |
| | MOTA | 17621 | CG1 | ILE | 2626 | 28.377 | 15.218 | 68.508 | 1.00 50.93 |
| | MOTA | 17622 | CD1 | ILE | 2626 | 29.050 | 16.524 | 68.131 | 1.00 51.04 |
| | ATOM | 17623 | C | ILE | 2626 | 28.494 | 12.335 | 67.984 | 1.00 47.86 |
| | ATOM | 17624 | 0 | ILE | 2626 | 28.875 | 12.067 | 69.122 | 1.00 47.90 |
| | ATOM | 17625 | N | PRO | 2627 | 29.189 | 11.963 | 66.899 | 1.00 45.93 |
| | ATOM | 17626 | CD | PRO | 2627 | 28.901 | 12.266 | 65.485 | 1.00 45.13 |
| | ATOM | 17627 | CA | PRO | 2627 | 30.436 | 11.203 | 67.026 | 1.00 43.64 |
| | ATOM | 17628 | CB | PRO | 2627 | 30.801 | 10.904 | 65.574 | 1.00 43.90 |
| | | | | | 2627 | 30.254 | 12.089 | 64.843 | 1.00 45.31 |
| | MOTA | 17629 17630 | CG | PRO | 2627 | 31.533 | 11.973 | 67.762 | 1.00 41.87 |
| | MOTA | | C | PRO | | | | | 1.00 41.57 |
| | MOTA | 17631 | 0 | PRO | 2627 | 31.599 | 13.198 | 67.687 | |
| | MOTA | 17632 | N | LYS | 2628 | 32.390 | 11.243 | 68.472 | 1.00 40.14 |
| | MOTA | 17633 | CA | LYS | 2628 | 33.486 | 11.846 | 69.224 | 1.00 39.09 |
| | MOTA | 17634 | CB | LYS | 2628 | 34.362 | 10.759 | 69.864 | 1.00 41.61 |
| | ATOM | 17635 | CG | LYS | 2628 | 34.081 | 10.500 | 71.340 | 1.00 44:14 |
| | MOTA | 17636 | CD | LYS | 2628 | 32.661 | 9.998 | 71.567 | |
| | MOTA | 17637 | CE | LYS | 2628 | 32.359 | 9.839 | 73.051 | 1.00 47.79 |
| | MOTA | 17638 | NZ | LYS | 2628 | 30.956 | 9.403 | 73.304 | 1.00 49.12 |
| | MOTA | 17639 | С | LYS | 2628 | 34.372 | 12.748 | 68.376 | 1.00 36.45 |
| | MOTA | 17640 | 0 | LYS | 2628 | 34.905 | 13.743 | 68.865 | 1.00 36.12 |
| | ATOM | 17641 | N | PHE | 2629 | 34.531 | 12.405 | 67.103 | 1.00 32.52 |
| | ATOM | 17642 | CA | PHE | 2629 | 35.387 | 13.189 | 66.224 | 1.00 29.15 |
| | ATOM | 17643 | CB | PHE | 2629 | 35.876 | 12.319 | 65.057 | 1.00 29.64 |
| | MOTA | 17644 | CG | PHE | 2629 | 34.772 | 11.753 | 64.216 | 1.00 29.08 |
| | | | | | 2629 | 34.772 | 12.561 | 63.328 | 1.00 29.61 |
| | MOTA | 17645 | | PHE | | | | | 1.00 29.81 |
| | ATOM | 17646 | | PHE | 2629 | 34.431 | 10.411 | 64.318 | |
| | MOTA | 17647 | | PHE | 2629 | 33.035 | 12.036 | 62.550 | 1.00 32.08 |
| | MOTA | 17648 | | PHE | 2629 | 33.403 | 9.873 | 63.550 | 1.00 32.17 |
| | MOTA | 17649 | cz | PHE | 2629 | 32.702 | 10.688 | 62.661 | 1.00 31.61 |
| | ATOM | 17650 | С | PHE | 2629 | 34.742 | 14.458 | 65.692 | 1.00 26.59 |
| | MOTA | 17651 | 0 | PHE | 2629 | 35.426 | 15.316 | 65.135 | 1.00 24.60 |
| | MOTA | 17652 | N | ALA | 2630 | 33.432 | 14.587 | 65.869 | 1.00 24.68 |
| | ATOM | 17653 | CA | ALA | 2630 | 32.720 | 15.764 | 65.388 | 1.00 24.35 |
| | ATOM | 17654 | CB | ALA | 2630 | 31.342 | 15.359 | 64.856 | 1.00 24.75 |
| | MOTA | 17655 | c | ALA | 2630 | 32.559 | 16.822 | 66.473 | 1.00 23.16 |
| | ATOM | 17656 | ō | ALA | 2630 | 32.719 | 16.539 | 67.659 | 1.00 23.58 |
| | MOTA | 17657 | N | LYS | 2631 | 32.713 | 18.043 | 66.046 | 1.00 23.38 |
| | | | | | | | 19.164 | 66.955 | 1.00 23.65 |
| | ATOM | 17658 | CA | LYS | 2631 | 32.039 | | | |
| | ATOM | 17659 | CB | LYS | 2631 | 33.319 | 19.993 | 67.105 | 1.00 23.84 |
| | ATOM | 17660 | CG | LYS | 2631 | 33.127 | 21.250 | 67.947 | 1.00 25.08 |
| | ATOM | 17661 | CD | LYS | 2631 | 34.435 | 21.990 | 68.159 | 1.00 25.96 |
| | | | | | | | | | |

| MOTA | 17662 | CE | LYS | 2631 | | 34.227 | 23.261 | 68.968 | 1.00 28.22 |
|--------------|----------------|------------|------------|---------------|---|------------------|------------------|---------------------------|--------------------------|
| MOTA | 17663 | NZ | LYS | 2631 | | 35.499 | 24.020 | 69.116 | 1.00 29.85 |
| MOTA | 17664 | C | LYS | 2631 | | 30.921 | 20.068 | 66.444 65.263 | 1.00 22.92 1.00 21.69 |
| MOTA | 17665 17666 | O N | LYS ASN | 2631 2632 | | 30.885 30.015 | 20.422 | 67.345 | 1.00 23.42 |
| ATOM ATOM | 17667 | CA | ASN | 2632 | | 28.889 | 21.310 | 67.026 | 1.00 22.87 |
| MOTA | 17668 | СВ | ASN | 2632 | | 27.771 | 21.121 | 68.058 | 1.00 22.06 |
| MOTA | 17669 | CG | ASN | 2632 | | 26.566 | 22.005 | 67.792 | 1.00 22.77 |
| MOTA | 17670 | | ASN | 2632 | | 26.626 | 22.943 | 66.994 | 1.00 23.52 |
| MOTA | 17671 | | ASN | 2632 | | 25.463 29.384 | 21.716 | 68. 4 75 67.080 | 1.00 20.23 1.00 22.32 |
| MOTA | 17672 17673 | C 0 | ASN ASN | 2632 2632 | | 29.559 | 22.748 23.306 | 68.167 | 1.00 22.04 |
| MOTA MOTA | 17674 | N | PHE | 2633 | | 29.617 | 23.348 | 65.918 | 1.00 20.88 |
| MOTA | 17675 | CA | PHE | 2633 | | 30.103 | 24.724 | 65.871 | 1.00 22.92 |
| ATOM | 17676 | CB | PHE | 2633 | | 30.879 | 24.987 | 64.576 | 1.00 23.76 |
| MOTA | 17677 | CG | PHE | 2633 | | 32.182 | 24.245 | 64.492 | 1.00 25.62 |
| MOTA | 17678 | CD1 | PHE | 2633 | | 32.224 | 22.938 | 64.020 | 1.00 25.78 1.00 25.99 |
| ATOM | 17679 | CD2 CE1 | PHE PHE | 2633 2633 | | 33.363 33.421 | 24.837 22.229 | 64.933 63.988 | 1.00 25.39 |
| MOTA MOTA | 17680 17681 | CE2 | PHE | 2633 | | 34.565 | 24.138 | 64.908 | 1.00 24.67 |
| ATOM | 17682 | CZ | PHE | 2633 | | 34.593 | 22.831 | 64.435 | 1.00 27.61 |
| ATOM | 17683 | С | PHE | 2633 | | 29.002 | 25.762 | 66.021 | 1.00 23.51 |
| MOTA | 17684 | 0 | PHE | 2633 | | 29.287 | 26.940 | 66.230 | 1.00 22.07 |
| ATOM | 17685 | N · | LEU | 2634 | | 27.748 | 25.329 | 65.917 | 1.00 23.90 1.00 25.40 |
| ATOM | 17686 | CA | LEU | 2634 2634 | | 26.625 25.351 | 26.246 25.628 | 66.056 65.485 | 1.00 23.46 |
| MOTA MOTA | 17687 17688 | CB CG | LEU | 2634 | | 24.073 | 26.438 | 65.713 | 1.00 19.60 |
| ATOM | 17689 | | LEU . | 2634 . | | 24.167 | 27.786 | 65.009 | 1.00 19.80 |
| ATOM | 17690 | CD2 | LEU | 2634 | - | 22.876 | 25.651 | 65.185 | 1.00 17.49 |
| MOTA | 17691 | C | LEU | 2634 | | 26.397 | 26.597 | 67.521 | 1.00 28.16 |
| MOTA | 17692 | 0 | LEU | 2634 | | 26.108 | 27.748 | 67.853 | 1.00 27.99 |
| MOTA | 17693 | N | ALA ALA | 2635 -2635 | | 26.516 26.326 | 25.592 25.760 | 68.384 69.820 | 1.00 30.92 1.00 36.08 |
| ATOM - | 17694 17695 | CA CB | ALA | 2635 | | 26.545 | 24.434 | 70.529 | 1.00 35.24 |
| ATOM | 17696 | C | ALA | 2635 | | 27.297 | 26.801 | 70.356 | 1.00 40.21 |
| ATOM | 17697 | 0 | ALA | 2635 | | 26.965 | 27.569 | 71.260 | 1.00 41.94 |
| MOTA | 17698 | N | GLU | 2636 | | 28.498 | 26.812 | 69.786 | 1.00 43.52 |
| MOTA | 17699 | CA | GLU | 2636 | | 29.550 | 27.748 | 70.170 | 1.00 47.26 |
| MOTA | 17700 | CB | GLU | 2636 | | 30.885 | 27.313 25.832 | 69.550 69.730 | 1.00 48.66 1.00 52.15 |
| ATOM ATOM | 17701 17702 | CG CD | GLU GLU | 2636 2636 | | 31.220 31.594 | 25.471 | 71.158 | 1.00 53.80 |
| ATOM | 17703 | OE1 | GLU | 2636 | | 30.830 | 25.815 | 72.085 | 1.00 55.93 |
| MOTA | 17704 | OE2 | GLU | 2636 | | 32.652 | 24.834 | 71.354 | 1.00 54.50 |
| MOTA | 17705 | С | GLU | 2636 | | 29.183 | 29.147 | 69.670 | 1.00 47.91 |
| ATOM | 17706 | 0 | GLU | 2636 | | 30.017 | 30.052 | 69.645 | 1.00 48.49 |
| ATOM | 17707 | N | THR | 2637 | | 27.927 27.418 | 29.306 30.575 | 69.263 68.764 | 1.00 48.71 1.00 48.27 |
| ATOM ATOM | 17708 17709 | CA CB | THR THR | 2637 2637 | | 28.031 | 30.914 | 67.384 | 1.00 48.89 |
| ATOM | 17710 | | THR | 2637 | | 27.518 | 32.171 | 66.927 | 1.00 48.26 |
| ATOM | 17711 | CG2 | THR | 2637 | | 27.693 | 29.833 | 66.365 | 1.00 49.85 |
| MOTA | 17712 | С | THR | 2637 | | 25.894 | 30.501 | 68.636 | 1.00 47.68 |
| MOTA | 17713 | 0 | THR | 2637 | | 25.236 | 29.744 | 69.356 | 1.00 48.21 |
| ATOM | 17714 | N | GLY | 2638 | | 25.336 23.898 | 31.289 31.283 | 67.724 67.526 | 1.00 45.54 1.00 43.10 |
| MOTA MOTA | 17715 17716 | CA ·· | GLY GLY | 2638 2638 | | 23.555 | 31.571 | 66.082 | 1.00 40.35 |
| ATOM | 17717 | o ` | GLY | 2638 | | 22.403 | 31.851 | 65.749 | 1.00 40.49 |
| ATOM | 17718 | N | ASP | 2639 | | 24.567 | 31.487 | 65.224 | 1.00 37.74 |
| ATOM | 17719 | CA | ASP | 2639 | | 24.411 | 31.755 | 63.799 | 1.00 35.76 |
| MOTA | 17720 | CB | ASP | 2639 | | 25.025 | 33.116 | 63.469 | 1.00 39.24 |
| ATOM | 17721 | CG | ASP | 2639 | | 24.688 25.570 | 33.573 34.144 | 62.078 61.405 | 1.00 41.90 1.00 42.76 |
| MOTA MOTA | 17722 17723 | | ASP ASP | 2639 2639 | | 23.576 | 33.367 | 61.662 | 1.00 46.27 |
| ATOM | 17724 | C | ASP | 2639 | | 25.110 | 30.676 | 62.967 | 1.00 32.25 |
| MOTA | 17725 | 0 | ASP | 2639 | | 26.276 | 30.361 | 63.206 | 1.00 30.44 |
| ATOM | 17726 | N | ILE | 2640 | | 24.409 | 30.119 | 61.985 | 1.00 28.72 |
| MOTA | 17727 | CA | ILE | 2640 | | 25.005 | 29.083 | 61.149 | 1.00 25.76 |
| ATOM | 17728 | CB | ILE | 2640 | | 23.959 | 28.470 27.628 | 60.176 59.111 | 1.00 25.25 1.00 23.48 |
| MOTA MOTA | 17729 17730 | CG2 CG1 | | 2640 2640 | | 24.657 22.952 | 27.628 | 60.969 | 1.00 23.48 |
| ATOM | 17731 | CD1 | | 2640 | | 21.751 | 27.150 | 60.161 | 1.00 23.27 |
| ATOM | 17732 | C | ILE | 2640 | | 26.204 | 29.612 | 60.358 | 1.00 25.06 |
| MOTA | 17733 | 0 | ILE | 2640 | | 27.251 | 28.963 | 60.299 | 1.00 25.46 |
| MOTA | 17734 | N | ARG | 2641 | | 26.061 | 30.785 | 59.752 | 1.00 24.74 |
| MOTA | 17735 | CA | ARG | 2641 | | 27.169 | 31.356 | 58.993 58.285 | 1.00 23.19 1.00 22.91 |
| ATOM - | 17736 17737 | CB CG | ARG ARG | 2641 2641 | | 26.739 25.858 | 32.642 32.392 | 57.077 | 1.00 22.91 |
| ATOM | 17738 | CD | ARG | 2641 | | 25.407 | 33.687 | 56.433 | 1.00 24.40 |
| | 250 | | | -011 | | , | / | | |

| ATOM | 17739 | NE | ARG | 2641 | 24.65 | 33.441 | 55.210 | 1.00 27.34 |
|--------------|----------------|--------|------------|--------------|----------------|----------|------------------|------------|
| ATOM | 17740 | CZ | ARG | 2641 | 23.45 | | 55.166 | 1.00 26.81 |
| ATOM | 17741 | NH1 | | 2641 | 22.85 | | 56.283 | 1.00 25.30 |
| ATOM | 17742 | NH2 | | 2641 | 22.85 | | 53.996 | 1.00 28.38 |
| | 17743 | C | ARG | 2641 | 28.34 | | 59.917 | 1.00 23.31 |
| MOTA | | | ARG | 2641 | 29.50 | | 59.511 | 1.00 20.74 |
| ATOM | 17744 | 0 | | 2642 | 28.04 | | 61.162 | 1.00 23.35 |
| MOTA | 17745 | N | ALA | | | | | 1.00 25.68 |
| ATOM | 17746 | CA | ALA | 2642 | 29.08 | | 62.143 | |
| MOTA | 17747 | CB | ALA | 2642 | 28.48 | | 63.404 | |
| MOTA | 17748 | C | ALA | 2642 | 29.76 | | 62.484 | 1.00 26.20 |
| MOTA | 17749 | 0 | ALA | 2642 | 30.97 | | 62.687 | 1.00 26.09 |
| ATOM | 17750 | N | ALA | 2643 | 28.97 | | 62.538 | 1.00 24.61 |
| MOTA | 17751 | CA | ALA | 2643 | 29.50 | | 62.847 | 1.00 24.08 |
| ATOM | 17752 | CB | ALA | 2643 | 28.36 | | 62.989 | 1.00 25.00 |
| ATOM | 17753 | С | ALA | 2643 | 30.46 | | 61.738 | 1.00 23.31 |
| MOTA | 17754 | 0 | ALA | 2643 | 31.49 | | 62.008 | 1.00 22.53 |
| MOTA | 17755 | N | VAL | 2644 | 30.10 | | 60.494 | 1.00 23.63 |
| MOTA | 17756 | CA | VAL | 2644 | 30.93 | | 59.340 | 1.00 23.56 |
| MOTA | 17757 | CB | VAL | 2644 | 30.26 | | 58.019 | 1.00 23.61 |
| ATOM | 17758 | CG1 | VAL | 2644 | 31.19 | | 56.850 | 1.00 23.86 |
| MOTA | 17759 | CG2 | VAL | 2644 | 28.95 | | 57.817 | 1.00 24.12 |
| MOTA | 17760 | С | VAL | 2644 | 32.28 | 7 28.762 | 59.443 | 1.00 25.21 |
| MOTA | 17761 | 0 | VAL | 2644 | 33.33 | 28.135 | 59.290 | 1.00 23.86 |
| MOTA | 17762 | N | ARG | 2645 | 32.25 | 7 30.066 | 59.689 | 1.00 24.95 |
| MOTA | 17763 | CA | ARG | 2645 | 33.47 | 30.846 | 59.828 | 1.00 27.28 |
| MOTA | 17764 | CB | ARG | 2645 | 33.13 | 32.318 | 60.084 | 1.00 27.82 |
| MOTA | 17765 | CG | ARG | 2645 | 32.44 | 33.015 | 58.922 | 1.00 28.30 |
| ATOM | 17766 | CD | ARG | 2645 | 32.29 | 4 34.509 | 59.187 | 1.00 32.06 |
| ATOM | 17767 | NE | ARG | 2645 | 31.36 | 1 34.790 | 60.279 | 1.00 34.28 |
| ATOM | 17768 | CZ | ARG | 2645 | 30.06 | 35.018 | 60.120 | 1.00 36.23 |
| ATOM | 17769 | NH1 | ARG | 2645 | 29.52 | 2 35.002 | 58.906 | 1.00 34.78 |
| ATOM | 17770 | NH2 | | 2645 | 29.29 | 7 35.265 | 61.177 | 1.00 37.25 |
| ATOM | 17771 | С | ARG | 2645 | 34.34 | | 60.970 | 1.00 27.28 |
| ATOM | 17772 | 0 | ARG | 2645 | 35.56 | 1 30.227 | 60.849 | 1.00 29.76 |
| ATOM | 17773 | N | GLN | 2646 | 33.70 | | 62.072 | 1.00 27.84 |
| ATOM | 17774 | CA | GLN | 2646 | 34.41 | | 63.233 | 1.00 27.15 |
| ATOM | 17775 | СВ | GLN | 2646 | 33.42 | | 64.384 | 1.00 31.32 |
| ATOM | 17776 | CG | GLN | 2646 | 34.08 | | 65.726 | 1.00 36.87 |
| ATOM | 17777 | CD | GLN | 2646 | 33.09 | | 66.757 | 1.00 41.60 |
| ATOM | 17778 | OE1 | | 2646 | 31.97 | | 66.878 | 1.00 45.33 |
| ATOM | 17779 | NE2 | GLN | 2646 | 33.50 | | 67.512 | 1.00 43.04 |
| ATOM | 17780 | C | GLN | 2646 | 35.10 | | 62.879 | 1.00 27.46 |
| ATOM | 17781 | ō | GLN | 2646 | 36.25 | | 63.275 | 1.00 24.55 |
| ATOM | 17782 | N | TYR | 2647 | 34.40 | | 62.135 | 1.00 24.93 |
| MOTA | 17783 | CA | TYR | 2647 | 34.94 | | 61.719 | 1.00 23.55 |
| ATOM | 17784 | CB | TYR | 2647 | 33.88 | | 60.934 | 1.00 22.15 |
| ATOM | 17785 | CG | TYR | 2647 | 34.39 | | 60.194 | 1.00 20.81 |
| ATOM | 17786 | CD1 | TYR | 2647 | 35.14 | | 60.848 | 1.00 22.12 |
| ATOM | 17787 | CE1 | TYR | 2647 | 35.59 | | 60.171 | 1.00 22.90 |
| ATOM | 17788 | CD2 | TYR | 2647 | 34.11 | | 58.846 | 1.00 21.36 |
| ATOM | 17789 | | TYR | 2647 | 34.55 | | 58.160 | 1.00 21.37 |
| | 17790 | CZ | TYR | 2647 | 35.29 | | 58.827 | 1.00 23.37 |
| ATOM | | OH | TYR | 2647 | 35.74 | | 58.149 | 1.00 23.07 |
| MOTA MOTA | 17791 | С | TYR | 2647 | 36.19 | | 60.861 | 1.00 23.07 |
| | 17792 | | | 2647 | 37.21 | | 61.064 | 1.00 22.24 |
| MOTA MOTA | 17793 17794 | O N | TYR MET | 2648 | 36.11 | | 59.909 | 1.00 22.24 |
| | 17795 | CA | MET | 2648 | 37.23 | | 59.023 | 1.00 23.34 |
| MOTA MOTA | 17796 | CB | MET | 2648 | 36.81 | | 57.968 | 1.00 24.40 |
| | | CG | MET | 2648 | 35.74 | | 57.000 | 1.00 25.72 |
| MOTA | 17797 | | | 2648 | 35.03 | | 56.049 | 1.00 29.67 |
| ATOM | 17798 | SD | MET MET | 2648 | 36.34 | | 54.905 | 1.00 29.14 |
| MOTA | 17799 | CE | | 2648 | 38.42 | | 59.816 | 1.00 25.14 |
| MOTA | 17800 | C | MET | | | | | 1.00 25.43 |
| ATOM | 17801 | O N | MET ALA | 2648 2649 | 39.57 38.13 | | 59.490 60.861 | 1.00 25.72 |
| ATOM | 17802 | | | | 39.18 | | | 1.00 25.72 |
| ATOM | 17803 | CA | ALA | 2649 2649 | 38.60 | | 61.690 62.575 | 1.00 23.41 |
| ATOM | 17804 | CB | ALA | | | | 62.552 | 1.00 25.43 |
| ATOM | 17805 | ·C | ALA | 2649 | 39.90 | | | |
| ATOM | 17806 | 0 | ALA | 2649 | 41.13 | | 62.557 | 1.00 25.14 |
| MOTA | 17807 | N | GLU | 2650 | 39.13 | | 63.280 | 1.00 25.28 |
| ATOM | 17808 | CA | GLU | 2650 | 39.71 | | 64.152 | 1.00 26.69 |
| MOTA | 17809 | CB | GLU | 2650 | 38.62 | | 64.981 | 1.00 28.05 |
| MOTA | 17810 | CG | GLU | 2650 | 38.20 | | 66.208 | 1.00 29.62 |
| ATOM | 17811 | CD | GLU | 2650 | 37.11 | | 67.014 | 1.00 29.84 |
| MOTA | 17812 | | GLU | 2650 | 37.15 | | 67.173 | 1.00 32.30 |
| MOTA | 17813 | | GLU | 2650 | 36.22 | | 67.506 | 1.00 33.86 |
| ATOM | | . c | GLU | 2650 | 40.53 | | | 1.00 26.90 |
| ATOM | 17815 | 0 | GLU | 2650 | 41.48 | 2 24.738 | 63.980 | 1.00 27.32 |
| | | | | | | | | |

| ATOM | 17816 | N | VAL | 2651 | 40.181 | 25.021 | 62.168 | 1.00 26.19 |
|------|-------|-----|----------------------|------|--------|--------|--------|------------|
| MOTA | 17817 | CA | VAL | 2651 | 40.914 | 24.042 | 61.380 | 1.00 25.27 |
| MOTA | 17818 | CB | VAL | 2651 | 40.163 | 23.681 | 60.078 | 1.00 24.96 |
| MOTA | 17819 | CG1 | VAL | 2651 | 41.063 | 22.849 | 59.179 | 1.00 23.48 |
| MOTA | 17820 | CG2 | VAL | 2651 | 38.891 | 22.900 | 60.411 | 1.00 23.49 |
| MOTA | 17821 | С | VAL | 2651 | 42.296 | 24.576 | 61.010 | 1.00 25.94 |
| ATOM | 17822 | 0 | VAL | 2651 | 43.279 | 23.836 | 61.032 | 1.00 25.81 |
| ATOM | 17823 | N | GLU | 2652 | 42.362 | 25.863 | 60.683 | 1.00 27.40 |
| ATOM | 17824 | CA | GLU | 2652 | 43.616 | 26.493 | 60.293 | 1.00 30.89 |
| ATOM | 17825 | CB | GLU | 2652 | 43.345 | 27.865 | 59.665 | 1.00 31.68 |
| ATOM | 17826 | CG | GLU | 2652 | 44.595 | 28.556 | 59.129 | 1.00 36.32 |
| ATOM | 17827 | CD | GLU | 2652 | 44.282 | 29.686 | 58.159 | 1.00 39.22 |
| ATOM | 17828 | | GLU | 2652 | 45.229 | 30.374 | 57.715 | 1.00 40.91 |
| ATOM | 17829 | OE2 | GLU | 2652 | 43.091 | 29.885 | 57.836 | 1.00 40.55 |
| ATOM | 17830 | C | GLU | 2652 | 44.614 | 26.638 | 61.438 | 1.00 32.09 |
| ATOM | 17831 | 0 | GLU | 2652 | 45.791 | 26.305 | 61.290 | 1.00 32.01 |
| ATOM | 17832 | N | SER | 2653 | 44.146 | 27.125 | 62.582 | 1.00 34.17 |
| ATOM | 17833 | CA | SER | 2653 | 45.026 | 27.310 | 63.727 | 1.00 36.02 |
| MOTA | 17834 | CB | SER | 2653 | 44.427 | 28.338 | 64.687 | 1.00 39.04 |
| ATOM | 17835 | OG | SER | 2653 | 44.357 | 29.613 | 64.066 | 1.00 44.62 |
| ATOM | 17836 | С | SER | 2653 | 45.317 | 26.001 | 64.454 | 1.00 35.06 |
| ATOM | 17837 | 0 | SER | 2653 | 46.243 | 25.923 | 65.262 | 1.00 36.58 |
| MOTA | 17838 | N | GLY | 2654 | 44.528 | 24.971 | 64.165 | 1.00 33.11 |
| MOTA | 17839 | CA | GLY | 2654 | 44.754 | 23.679 | 64.789 | 1.00 29.91 |
| MOTA | 17840 | С | GLY | 2654 | 43.918 | 23.352 | 66.012 | 1.00 27.78 |
| ATOM | 17841 | 0 | GLY | 2654 | 44.111 | 22.302 | 66.625 | 1.00 30.35 |
| ATOM | 17842 | N | VAL | 2655 | 42.999 | 24.239 | 66.376 | 1.00 26.05 |
| MOTA | 17843 | CA | VAL | 2655 | 42.129 | 24.020 | 67.529 | 1.00 24.30 |
| ATOM | 17844 | CB | VAL | 2655 | 41.290 | 25.277 | 67.832 | 1.00 25.65 |
| ATOM | 17845 | CG1 | VAL | 2655 | 40.191 | 24.946 | 68.833 | 1.00 27.96 |
| MOTA | 17846 | CG2 | VAL | 2655 | 42.196 | 26.371 | 68.399 | 1.00 26.98 |
| MOTA | 17847 | С | VAL | 2655 | 41.190 | 22.839 | 67.288 | 1.00 23.05 |
| ATOM | 17848 | 0 | VAL | 2655 | 40.821 | 22.125 | 68.221 | 1.00 19.84 |
| MOTA | 17849 | N | TYR | 2656 | 40.807 | 22.644 | 66.030 | 1.00 23.31 |
| ATOM | 17850 | CA | TYR | 2656 | 39.926 | 21.541 | 65.659 | 1.00 23.29 |
| ATOM | 17851 | CB | TYR | 2656 | 38.554 | 22.054 | 65.203 | 1.00 24.58 |
| ATOM | 17852 | CG | TYR | 2656 | 37.625 | 20.927 | 64.795 | 1.00 26.25 |
| ATOM | 17853 | CD1 | TYR | 2656 | 37.053 | 20.092 | 65.755 | 1.00 26.34 |
| ATOM | 17854 | CE1 | TYR | 2656 | 36.272 | 19.000 | 65.389 | 1.00 27.58 |
| ATOM | 17855 | CD2 | TYR | 2656 | 37.384 | 20.646 | 63.450 | 1.00 26.60 |
| ATOM | 17856 | CE2 | TYR | 2656 | 36.602 | 19.553 | 63.069 | 1.00 26.50 |
| MOTA | 17857 | CZ | TYR | 2656 | 36.052 | 18.734 | 64.048 | 1.00 28.77 |
| ATOM | 17858 | OH | TYR | 2656 | 35.298 | 17.633 | 63.693 | 1.00 29.76 |
| ATOM | 17859 | С | TYR | 2656 | 40.539 | 20.739 | 64.520 | 1.00 22.07 |
| ATOM | 17860 | 0 | TYR | 2656 | 40.971 | 21.308 | 63.519 | 1.00 21.40 |
| MOTA | 17861 | N | PRO | 2657 | 40.575 | 19.407 | 64.659 | 1.00 23.11 |
| MOTA | 17862 | CD | PRO | 2657 | 40.839 | 18.474 | 63.551 | 1.00 25.30 |
| MOTA | 17863 | CA | PRO | 2657 | 40.064 | 18.682 | 65.827 | 1.00 25.15 |
| ATOM | 17864 | CB | PRO | 2657 | 39.863 | 17.266 | 65.293 | 1.00 25.49 |
| ATOM | 17865 | CG | PRO | 2657 | 40.930 | 17.153 | 64.267 | 1.00 26.67 |
| MOTA | 17866 | С | PRO | 2657 | 40.987 | 18.704 | 67.047 | 1.00 26.33 |
| MOTA | 17867 | 0 | PRO | 2657 | 42.194 | 18.937 | 66.934 | 1.00 24.35 |
| MOTA | 17868 | N | GLY | 2658 | 40.402 | 18.451 | 68.212 | 1.00 28.19 |
| ATOM | 17869 | CA | GLY | 2658 | 41.175 | 18.424 | 69.435 | 1.00 29.27 |
| MOTA | 17870 | С | GLY | 2658 | 41.405 | 16.990 | 69.870 | 1.00 31.45 |
| MOTA | 17871 | 0 | GLY | 2658 | 41.011 | 16.048 | 69.175 | 1.00 29.26 |
| ATOM | 17872 | N | GLU | 2659 | 42.039 | 16.825 | 71.025 | 1.00 31.72 |
| ATOM | 17873 | CA | GLU | 2659 | 42.328 | 15.506 | 71.568 | 1.00 33.60 |
| MOTA | 17874 | CB | GLU | 2659 | 43.166 | 15.638 | 72.845 | 1.00 35.63 |
| MOTA | 17875 | CG | GLU | 2659 | 43.629 | 14.310 | 73.412 | 1.00 38.07 |
| MOTA | 17876 | CD | GLU | 2659 | 44.583 | 13.585 | 72.476 | 1.00 40.89 |
| MOTA | 17877 | OE1 | | 2659 | 44.763 | 12.360 | 72.642 | 1.00 41.36 |
| MOTA | 17878 | OE2 | | 2659 | 45.156 | 14.245 | 71.582 | 1.00 41.02 |
| MOTA | 17879 | С | GLU | 2659 | 41.043 | 14.746 | 71.874 | 1.00 33.45 |
| ATOM | 17880 | 0 | GLU | 2659 | 41.012 | 13.514 | 71.823 | 1.00 33.66 |
| MOTA | 17881 | N | GLU | 2660 | 39.981 | 15.484 | 72.193 | 1.00 34.34 |
| ATOM | 17882 | CA | GLU | 2660 | 38.692 | 14.869 | 72.507 | 1.00 34.69 |
| MOTA | 17883 | CB | GLU | 2660 | 37.738 | 15.890 | 73.136 | 1.00 36.58 |
| MOTA | 17884 | CG | GLU | 2660 | 38.416 | 17.063 | 73.818 | 1.00 41.62 |
| MOTA | 17885 | CD | GLU | 2660 | 38.836 | 18.147 | 72.839 | 1.00 43.50 |
| MOTA | 17886 | | GLU | 2660 | 37.945 | 18.737 | 72.186 | 1.00 43.66 |
| MOTA | 17887 | OE2 | | 2660 | 40.055 | 18.409 | 72.727 | 1.00 44.50 |
| ATOM | 17888 | С | GLU | 2660 | 38.057 | 14.328 | 71.233 | 1.00 33.13 |
| MOTA | 17889 | 0 | GLU | 2660 | 37.165 | 13.482 | 71.287 | 1.00 33.50 |
| MOTA | 17890 | N | HIS. | 2661 | 38.526 | 14.827 | 70.093 | 1.00 31.20 |
| MOTA | 17891 | CA | HIS | 2661 | 38.010 | 14.415 | 68.792 | 1.00 29.37 |
| MOTA | 17892 | CB | HIS | 2661 | 37.777 | 15.643 | 67.903 | 1.00 29.29 |

| ATOM | 17893 | CG | HIS | 2661 | 36.937 | 16.708 | 68.537 | 1.00 29.26 |
|--------------|----------------|-----------|----------------|--------------|------------------|------------------|------------------|--------------------------|
| ATOM | 17894 | | HIS | 2661 | 37.231 | 17.984 | 68.884 | 1.00 28.56 |
| MOTA | 17895 | | HIS | 2661 | 35.613 | 16.517 | 68.868 | 1.00 29.92 |
| ATOM | 17896 | | HIS | 2661 | 35.126 | 17.630 | 69.391 | 1.00 29.59 |
| ATOM | 17897 | NE2 | | 2661 | 36.088 | 18.535 | 69.411 | 1.00 28.86 |
| ATOM | 17898 | С | HIS | 2661 | 38.983 | 13.480 | 68.076 | 1.00 28.74 |
| ATOM | 17899 | ō | HIS | 2661 | 38.755 | 13.119 | 66.924 | 1.00 28.41 |
| ATOM | 17900 | N | SER | 2662 | 40.055 | 13.088 | 68.761 | 1.00 27.65 |
| ATOM | 17901 | CA | SER | 2662 | 41.077 | 12.226 | 68.171 | 1.00 27.75 |
| ATOM | 17902 | CB | SER | 2662 | 42.453 | 12.873 | 68.346 | 1.00 24.62 |
| ATOM | 17903 | OG | SER | 2662 | 42.507 | 14.139 | 67.714 | 1.00 24.83 |
| ATOM | 17904 | С | SER | 2662 | 41.128 | 10.800 | 68.711 | 1.00 27.87 |
| MOTA | 17905 | 0 | SER | 2662 | 40.798 | 10.541 | 69.872 | 1.00 28.57 |
| ATOM | 17906 | N | PHE | 2663 | 41.562 | 9.876 | 67.857 | 1.00 27.35 |
| ATOM | 17907 | CA | PHE | 2663 | 41.680 | 8.472 | 68.231 | 1.00 27.58 |
| ATOM | 17908 | СВ | PHE | 2663 | 40.990 | 7.581 | 67.195 | 1.00 28.72 |
| MOTA | 17909 | CG | PHE | 2663 | 39.507 | 7.795 | 67.099 | 1.00 28.64 |
| MOTA | 17910 | CD1 | | 2663 | 38.948 | 8.405 | 65.980 | 1.00 28.22 |
| ATOM | 17911 | CD2 | | 2663 | 38.664 | 7.369 | 68.123 | 1.00 28.60 |
| ATOM | 17912 | CE1 | PHE | 2663 | 37.568 | 8.585 | 65.879 | 1.00 28.53 |
| ATOM | 17913 | CE2 | PHE | 2663 | 37.284 | 7.545 | 68.033 | 1.00 28.38 |
| ATOM | 17914 | CZ | PHE | 2663 | 36.736 | 8.152 | 66.909 | 1.00 27.60 |
| ATOM | 17915 | С | PHE | 2663 | 43.147 | 8.070 | 68.337 | 1.00 29.19 |
| MOTA | 17916 | 0 | PHE | 2663 | 44.009 | 8.662 | 67.693 | 1.00 28.67 |
| MOTA | 17917 | N | HIS | 2664 | 43.425 | 7.061 | 69.154 | 1.00 30.62 |
| ATOM | 17918 | CA | HIS | 2664 | 44.793 | 6.580 | 69.335 | 1.00 33.11 |
| ATOM | 17919 | CB | HIS | 2664 | 45.390 | 7.136 | 70.631 | 1.00 32.47 |
| ATOM | 17920 | CG | HIS | 2664 | 45.696 | 8.600 | 70.569 | 1.00 31.82 |
| MOTA | 17921 | CD2 | HIS | 2664 | 45.143 | 9.657 | 71.209 | 1.00 31.31 |
| MOTA | 17922 | ND1 | HIS | 2664 | 46.670 | 9.119 | 69.743 | 1.00 31.66 |
| MOTA | 17923 | CE1 | HIS | 2664 | 46.704 | 10.433 | 69.877 | 1.00 32.26 |
| ATOM | 17924 | NE2 | HIS | 2664 | 45.787 | 10.785 | 70.761 | 1.00 31.44 |
| MOTA | 17925 | C | HIS | 2664 | 44.850 | 5.060 | 69.347 | 1.00 34.16 |
| MOTA | 17926 | O | HIS | 2664 | 45.924 | 4.517 | 69.013 | 1.00 34.77 |
| MOTA | 17927 | OXT | HIS | 2664 | 43.825 | 4.436 | 69.698 | 1.00 34.27 |
| MOTA | 17928 | C1 | KPL | 2665 | 32.243 | 11.877 | 55.862 | 1.00 40.79 |
| MOTA | 17929 | C2 | KPL | 2665 | 32.961 | 11.755 | 54.501 | 1.00 41.02 |
| ATOM | 17930 | C3 | KPL | 2665 | 33.077 | 13.146 | 53.870 | 1.00 41.20 |
| ATOM | 17931 | C4 | KPL | 2665 | 34.387 | 11.202 | 54.712 | 1.00 42.66 |
| MOTA | 17932 | 01 | KPL | 2665 | 34.336 | 9.899 | 55.310 | 1.00 45.13 |
| MOTA | 17933 | C5 | KPL | 2665 | 32.150 | 10.836 | 53.550 | 1.00 39.59 |
| MOTA | 17934 | 02 | KPL | 2665 | 32.663 | 9.838 | 53.081 | 1.00 38.96 |
| MOTA | 17935 | C6 | KPL | 2665 | 30.715 | 11.146 | 53.180 | 1.00 37.68 |
| MOTA | 17936 | 03 | \mathtt{KPL} | 2665 | 30.159 | 12.135 | 53.620 | 1.00 35.87 |
| MOTA | 17937 | 04 | KPL | 2665 | 30.039 | 10.319 | 52.357 | 1.00 34.01 |
| MOTA | 17938 | CB | MET | 2701 | 34.899 | 19.058 | -4.231 | 1.00 73.64 |
| MOTA | 17939 | CG | MET | 2701 | 35.731 | 17.961 | -3.594 | 1.00 74.75 |
| MOTA | 17940 | SD | MET | 2701 | 37.148 | 17.478 | -4.583 | 1.00 76.63 |
| MOTA | 17941 | CE | MET | 2701 | 36.494 | 16.017 | -5.398 | 1.00 76.51 |
| ATOM | 17942 | С | MET | 2701 | 32.655 | 18.015 | -4.580 | 1.00 71.20 |
| MOTA | 17943 | 0 | MET | 2701 | 31.627 | 18.329 | -5.182 | 1.00 71.65 |
| ATOM | 17944 | N | MET | 2701 | 33.341 | 18.824 | -2.319 | 1.00 71.84 |
| MOTA | 17945 | CA | MET | 2701 | 33.434 | 19.060 | -3.787 | 1.00 72.13 |
| MOTA | 17946 | N | LYS | 2702 | 33.136 | 16.777 | -4.578 | 1.00 69.46 |
| MOTA | 17947 | CA | LYS | 2702 | 32.480 | 15.710 | -5.314 | 1.00 67.58 |
| ATOM | 17948 | CB | LYS | 2702 | 33.180 | 15.500 | -6.657 | 1.00 68.24 |
| ATOM | 17949 | CG | LYS | 2702 | 33.257 | 16.745 | -7.532 | 1.00 69.09 |
| MOTA | 17950 | CD | LYS | 2702 | 31.884 | 17.196 | -8.031 | 1.00 69.83 |
| ATOM | 17951 | CE | LYS | 2702 | 31.288 | 16.208 | -9.025 | 1.00 70.29 |
| ATOM | 17952 | NZ | LYS | 2702 | 29.978 | 16.690 | -9.549 | 1.00 70.64 |
| ATOM | 17953 | C | LYS | 2702 | 32.359 | 14.356 | -4.586 | 1.00 65.56 |
| ATOM | 17954 | 0 | LYS | 2702 | 32.309 | 13.312 | -5.230 | 1.00 66.40 |
| ATOM | 17955 | N | PRO | 2703 | 32.359 | 14.356 | -3.236 | 1.00 62.79 |
| ATOM | 17956 | CD | PRO | 2703 | 31.899 | 13.174 | -2.477 | 1.00 62.15 |
| MOTA | 17957 | CA | PRO | 2703 | 32.399 | 15.527 | -2.353 | 1.00 60.20 |
| MOTA | 17958 | CB | PRO | 2703 | 31.472 | 15.124 | -1.221 | 1.00 60.98 |
| ATOM | 17959 | CG | PRO | 2703 | 31.824 | 13.700 | -1.045 | 1.00 61.24 |
| ATOM | 17960 | C | PRO | 2703 | 33.838 | 15.784 | -1.867 | 1.00 57.10 |
| ATOM | 17961 | 0 | PRO | 2703 | 34.808 | 15.402 | -2.523 | 1.00 56.61 |
| ATOM | 17962 | N | THR | 2704 | 33.954 | 16.429 | -0.711 -0.126 | 1.00 54.53 |
| MOTA | 17963 | CA | THR | 2704 | 35.261 | 16.729 | -0.126 | 1.00 51.38 |
| ATOM | 17964 | CB OC1 | THR | 2704 | 35.267 | 18.095 | 0.603 | 1.00 51.73 1.00 52.06 |
| ATOM ATOM | 17965 17966 | | THR | 2704 | 34.978 36.630 | 19.147 18.346 | -0.328 1.240 | 1.00 52.06 |
| ATOM | 17966 | | THR | 2704 | 35.628 | 18.346 | 0.884 | 1.00 50.43 |
| ATOM | 17967 | С 0 | THR THR | 2704 2704 | 35.028 | 15.571 | 1.963 | 1.00 49.86 |
| ATOM | 17969 | N | THR | 2704 | 36.605 | 14.819 | 0.532 | 1.00 48.30 |
| 111 OF1 | 1,202 | TA | TUK | 2703 | 50.005 | 14.U17 | 0.334 | 1.00 40.07 |

| MOTA | 17970 | CA | THR | 2705 | 37.040 | 13.743 | 1.410 | 1.00 47.18 |
|------|-------|-----|-------|------|------------------|------------------|--------|------------|
| ATOM | 17971 | CB | THR | 2705 | 37.087 | 12.397 | 0.664 | 1.00 46.54 |
| ATOM | 17972 | OG1 | THR | 2705 | 38.071 | 12.459 | -0.375 | 1.00 45.99 |
| ATOM | 17973 | CG2 | THR | 2705 | 35.728 | 12.081 | 0.051 | 1.00 46.51 |
| | 17974 | C | THR | 2705 | 38.422 | 14.017 | 1.995 | 1.00 46.48 |
| ATOM | | | THR | 2705 | 39.061 | 15.016 | 1.664 | 1.00 45.98 |
| MOTA | 17975 | 0 | | | 38.875 | 13.119 | 2.864 | 1.00 45.87 |
| ATOM | 17976 | N | ILE | 2706 | | | | 1.00 45.37 |
| ATOM | 17977 | CA | ILE | 2706 | 40.180 | 13.245 | 3.502 | |
| MOTA | 17978 | CB | ILE | 2706 | 40.461 | 12.049 | 4.438 | 1.00 45.76 |
| ATOM | 17979 | CG2 | ILE | 2706 | 41.744 | 12.292 | 5.223 | 1.00 45.05 |
| MOTA | 17980 | CG1 | ILE | 2706 | 39.287 | 11.852 | 5.400 | 1.00 47.29 |
| MOTA | 17981 | CD1 | ILE | 2706 | 39.380 | 10.579 | 6.232 | 1.00 47.98 |
| MOTA | 17982 | С | ILE | 2706 | 41.278 | 13.293 | 2.443 | 1.00 45.82 |
| ATOM | 17983 | 0 | ILE | 2706 | 42.361 | 13.834 | 2.676 | 1.00 44.79 |
| ATOM | 17984 | N | SER | 2707 | 40.992 | 12.719 | 1.278 | 1.00 45.94 |
| MOTA | 17985 | CA | SER | 2707 | 41.949 | 12.697 | 0.174 | 1.00 46.20 |
| ATOM | 17986 | CB | SER | 2707 | 41.338 | 11.997 | -1.045 | 1.00 46.03 |
| ATOM | 17987 | OG | SER | 2707 | 41.014 | 10.650 | -0.758 | 1.00 47.96 |
| ATOM | 17988 | C | SER | 2707 | 42.380 | 14.110 | -0.214 | 1.00 45.55 |
| ATOM | 17989 | Ō | SER | 2707 | 43.555 | 14.357 | -0.489 | 1.00 44.61 |
| ATOM | 17990 | N | LEU | 2708 | 41.423 | 15.032 | -0.236 | 1.00 45.78 |
| ATOM | 17991 | CA | LEU | 2708 | 41.699 | 16.422 | -0.590 | 1.00 46.61 |
| MOTA | 17992 | CB | LEU | 2708 | 40.410 | 17.250 | -0.538 | 1.00 47.45 |
| ATOM | 17993 | CG | LEU | 2708 | 39.904 | 17.852 | -1.853 | 1.00 47.62 |
| | 17994 | | LEU | 2708 | 38.612 | 18.619 | -1.609 | 1.00 48.54 |
| ATOM | 17995 | | | 2708 | 40.960 | 18.772 | -2.436 | 1.00 48.50 |
| ATOM | | | LEU | | | | 0.333 | 1.00 46.79 |
| MOTA | 17996 | C | LEU | 2708 | 42.741 43.699 | 17.051 17.671 | | 1.00 46.73 |
| ATOM | 17997 | 0 . | LEU | 2708 | | | -0.133 | |
| MOTA | 17998 | N | LEU | 2709 | 42.549 | 16.890 | 1.640 | |
| MOTA | 17999 | CA | LEU | 2709 | 43.469 | 17.452 | 2.626 | 1.00 48.38 |
| MOTA | 18000 | CB | LEU | 2709 | 42.935 | 17.231 | 4.044 | 1.00 47.81 |
| MOTA | 18001 | CG | LEU | 2709 | 41.545 | 17.782 | 4.367 | 1.00 48.04 |
| MOTA | 18002 | | LEU | 2709 | 41.209 | 17.497 | 5.827 | 1.00 46.71 |
| MOTA | 18003 | CD2 | LEU | 2709 | 41.510 | 19.276 | 4.098 | 1.00 48.90 |
| MOTA | 18004 | С | LEU | 2709 | 44.854 | 16.829 | 2.505 | 1.00 49.28 |
| ATOM | 18005 | 0 | LEU | 2709 | 45.861 | 17.455 | 2.835 | 1.00 48.60 |
| MOTA | 18006 | N | GLN | 2710 | 44.895 | 15.589 | 2.032 | 1.00 50.99 |
| MOTA | 18007 | CA | GLN | 2710 | 46.154 | 14.880 | 1.867 | 1.00 52.96 |
| MOTA | 18008 | СВ | GLN | 2710 | 45.893 | 13.391 | 1.632 | 1.00 54.28 |
| ATOM | 18009 | CG | GLN | 2710 | 47.137 | 12.520 | 1.688 | 1.00 57.12 |
| ATOM | 18010 | CD | GLN | 2710 | 47.721 | 12.419 | 3.087 | 1.00 58.97 |
| ATOM | 18011 | OE1 | GLN | 2710 | 48.102 | 13.423 | 3.692 | 1.00 60.04 |
| MOTA | 18012 | NE2 | | 2710 | 47.794 | 11.198 | 3.607 | 1.00 59.77 |
| ATOM | 18013 | C | GLN | 2710 | 46.909 | 15.476 | 0.683 | 1.00 53.46 |
| ATOM | 18014 | O | GLN | 2710 | 48.096 | 15.790 | 0.787 | 1.00 53.06 |
| АТОМ | 18015 | N | LYS | 2711 | 46.214 | 15.635 | -0.441 | 1.00 53.98 |
| MOTA | 18016 | CA | LYS | 2711 | 46.824 | 16.205 | -1.636 | 1.00 54.78 |
| ATOM | 18017 | CB | LYS | 2711 | 45.817 | 16.278 | -2.789 | 1.00 55.24 |
| ATOM | 18018 | CG | LYS | 2711 | 46.421 | 16.833 | -4.076 | 1.00 55.62 |
| ATOM | 18019 | CD | LYS | 2711 | 45.396 | 17.536 | -4.955 | 1.00 57.13 |
| | 18020 | CE | LYS | 2711 | 44.346 | 16.586 | -5.502 | 1.00 57.37 |
| ATOM | 18020 | NZ | LYS | 2711 | 43.404 | 17.307 | -6.407 | |
| ATOM | | | | | 47.318 | 17.614 | -1.332 | 1.00 54.66 |
| MOTA | 18022 | C | LYS | 2711 | 48.382 | 18.025 | -1.792 | 1.00 55.31 |
| ATOM | 18023 | 0 | LYS | 2711 | | | -0.558 | 1.00 54.70 |
| ATOM | 18024 | N | TYR | 2712 | 46.531 | 18.354 | | 1.00 54.60 |
| ATOM | 18025 | CA | TYR | 2712 | 46.881 | 19.721 | -0.193 | 1.00 54.84 |
| ATOM | 18026 | CB | TYR | 2712 | 45.796 | 20.328 | 0.698 | |
| ATOM | 18027 | CG | TYR | 2712 | 44.590 | 20.842 | -0.059 | 1.00 55.24 |
| ATOM | 18028 | | TYR | 2712 | 43.480 | 21.344 | 0.620 | 1.00 55.21 |
| ATOM | 18029 | | TYR | 2712 | 42.375 | 21.837 | -0.071 | 1.00 55.78 |
| MOTA | 18030 | | TYR | 2712 | 44.564 | 20.847 | -1.456 | 1.00 55.42 |
| MOTA | 18031 | CE2 | TYR | 2712 | 43.465 | 21.338 | -2.155 | 1.00 55.89 |
| ATOM | 18032 | CZ | TYR | 2712 | 42.376 | 21.830 | -1.458 | 1.00 55.09 |
| MOTA | 18033 | ОН | TYR | 2712 | 41.290 | 22.313 | -2.145 | 1.00 55.85 |
| MOTA | 18034 | С | TYR | 2712 | 48.227 | 19.825 | 0.505 | 1.00 54.49 |
| ATOM | 18035 | 0 | TYR | 2712 | 49.023 | 20.709 | 0.191 | 1.00 54.80 |
| MOTA | 18036 | N | LYS | 2713 | 48.485 | 18.928 | 1.450 | 1.00 54.67 |
| ATOM | 18037 | CA | LYS | 2713 | 49.747 | 18.958 | 2.175 | 1.00 55.19 |
| MOTA | 18038 | CB | LYS | 2713 | 49.787 | 17.860 | 3.241 | 1.00 53.74 |
| MOTA | 18039 | ĊG | LYS | 2713 | 51.072 | | 4.056 | 1.00 52.19 |
| ATOM | 18040 | CD | LYS | 2713 | 50.915 | 17.134 | 5.372 | 1.00 50.87 |
| ATOM | 18041 | CE | LYS | 2713 | 52.169 | 17.275 | 6.218 | 1.00 50.54 |
| ATOM | 18042 | NZ | LYS | 2713 | 51.974 | 16.777 | 7.605 | 1.00 49.42 |
| ATOM | 18043 | C | LYS | 2713 | 50.935 | 18.809 | 1.232 | 1.00 55.89 |
| ATOM | 18044 | 0 | LYS | 2713 | 51.998 | 19.380 | 1.471 | 1.00 56.25 |
| ATOM | 18045 | N | GLN | 2714 | 50.753 | 18.042 | 0.161 | 1.00 57.18 |
| ATOM | 18046 | CA | GLN | 2714 | 51.820 | 17.844 | -0.812 | 1.00 58.36 |
| 011 | T0040 | | ~1114 | | 31.020 | | | |

| ATOM | 18047 | СВ | GLN | 2714 | 51.438 | 16.763 | -1.819 | 1.00 59.42 |
|------|-------|------|-----|------------------|--------|--------|----------------|------------|
| ATOM | 18048 | CG | GLN | 2714 | 51.254 | 15.390 | -1.216 | 1.00 61.57 |
| ATOM | 18049 | CD | GLN | 2714 | 50.997 | | -2.270 | 1.00 62.96 |
| | | OE1 | | 2714 | 51.813 | 14.134 | -3.171 | 1.00 64.00 |
| ATOM | 18050 | | | | 49.859 | | -2.166 | |
| ATOM | 18051 | | GLN | 2714 | | 13.656 | | 1.00 63.63 |
| MOTA | 18052 | С | GLN | 2714 | 52.073 | 19.146 | -1.551 | 1.00 58.50 |
| MOTA | 18053 | Ο ,, | GLN | 2714 | 53.217 | 19.563 | -1.722 | 1.00 59.24 |
| ATOM | 18054 | N | GLU | 2715 | 50.992 | 19.785 | -1.986 | 1.00 58.54 |
| MOTA | 18055 | CA | GLU | 2715 | 51.082 | 21.042 | -2.714 | 1.00 58.89 |
| ATOM | 18056 | CB | GLU | 2715 | 49.783 | 21.294 | -3.477 | 1.00 59.02 |
| MOTA | 18057 | CG | GLU | 2715 | 49.372 | 20.144 | -4.373 | 1.00 59.98 |
| ATOM | 18058 | CD | GLU | 2715 | 48.032 | 20.381 | -5.034 | 1.00 60.87 |
| ATOM | 18059 | OE1 | GLU | 2715 | 47.061 | 20.683 | -4.309 | 1.00 61.95 |
| ATOM | 18060 | OE2 | GLU | 2715 | 47.946 | 20.260 | -6.274 | 1.00 61.16 |
| ATOM | 18061 | C | GLU | 2715 | 51.352 | 22.199 | -1.761 | 1.00 58.97 |
| MOTA | 18062 | ō | GLU | 2715 | 51.366 | 23.360 | -2.169 | 1.00 59.41 |
| ATOM | 18063 | N | LYS | 2716 | 51.563 | 21.874 | -0.489 | 1.00 58.61 |
| | 18064 | CA | LYS | 2716 | 51.836 | 22.882 | 0.531 | 1.00 58.78 |
| MOTA | | | | | 53.169 | 23.578 | 0.331 | 1.00 58.70 |
| MOTA | 18065 | CB | LYS | 2716 | | | | |
| MOTA | 18066 | CG | LYS | 2716 | 54.325 | 22.634 | -0.032 | 1.00 59.65 |
| MOTA | 18067 | CD | LYS | 2716 | 54.665 | 21.785 | 1.178 | 1.00 60.37 |
| MOTA | 18068 | CE | LYS | 2716 | 55.783 | 20.805 | 0.853 | 1.00 61.03 |
| MOTA | 18069 | NZ | LYS | 2716 | 57.003 | 21.501 | 0.359 | 1.00 60.83 |
| ATOM | 18070 | С | LYS | 2716 | 50.722 | 23.924 | 0.561 | 1.00 58.16 |
| MOTA | 18071 | 0 | LYS | 2716 | 50.926 | 25.047 | 1.020 | 1.00 58.70 |
| MOTA | 18072 | N | LYS | 2717 | 49.548 | 23.544 | 0.065 | 1.00 57.44 |
| ATOM | 18073 | CA | LYS | 2717 | 48.400 | 24.442 | 0.024 | 1.00 56.21 |
| ATOM | 18074 | СВ | LYS | 2717 | 47.502 | 24.083 | -1.167 | 1.00 57.20 |
| ATOM | 18075 | CG | LYS | 2717 | 46.344 | 25.048 | -1.400 | 1.00 58.48 |
| MOTA | 18076 | CD | LYS | 2717 | 45.574 | 24.717 | -2.679 | 1.00 59.26 |
| ATOM | 18077 | CE | LYS | 2717 | 46.441 | 24.883 | -3.925 | 1.00 60.27 |
| ATOM | 18078 | NZ | LYS | 2717 | 45.681 | 24.594 | -5.174 | 1.00 59.88 |
| | | - | | | | | 1.326 | 1.00 55.15 |
| ATOM | 18079 | C | LYS | 2717 | 47.604 | 24.368 | | |
| MOTA | 18080 | 0 | LYS | 2717 | 46.819 | 23.443 | 1.536 | 1.00 55.14 |
| MOTA | 18081 | N | ARG | 2718 | 47.820 | 25.350 | 2.197 | 1.00 53.27 |
| MOTA | 18082 | CA | ARG | 2718 | 47.135 | 25.413 | 3.483 | 1.00 52.15 |
| MOTA | 18083 | CB | ARG | 2718 | 47.728 | | 4.334 | 1.00 52.42 |
| ATOM | 18084 | CG | ARG | 2718 | 49.122 | 26.226 | 4.849 | 1.00 53.20 |
| MOTA | 18085 | CD | ARG | 2718 | 49.749 | 27.416 | 5.548 | 1.00 54.76 |
| ATOM | 18086 | NE | ARG | 2718 | 50.135 | 28.463 | 4.605 | 1.00 55.74 |
| ATOM | 18087 | CZ | ARG | 2718 | 50.810 | 29.557 | 4.944 | 1.00 56.58 |
| ATOM | 18088 | NH1 | ARG | 2718 | 51.173 | 29.750 | 6.204 | 1.00 56.22 |
| ATOM | 18089 | NH2 | | 2718 | 51.131 | 30.454 | 4.021 | 1.00 57.45 |
| ATOM | 18090 | C | ARG | 2718 | 45.632 | 25.612 | 3.328 | 1.00 50.84 |
| ATOM | 18091 | ō | ARG | 2718 | 45.182 | 26.468 | 2.565 | 1.00 50.29 |
| ATOM | 18092 | N | PHE | 2719 | 44.863 | 24.816 | 4.067 | 1.00 48.72 |
| ATOM | 18093 | CA | PHE | 2719 | 43.406 | 24.872 | 4.016 | 1.00 46.09 |
| | | | | | | 23.483 | 3.674 | 1.00 47.13 |
| ATOM | 18094 | CB | PHE | 2719 | 42.856 | | | |
| MOTA | 18095 | CG | PHE | 2719 | 43.372 | 22.390 | 4.565 | 1.00 46.19 |
| MOTA | 18096 | | PHE | 2719 | 42.764 | 22.122 | 5.788 | 1.00 46.63 |
| ATOM | 18097 | | PHE | 2719 | 44.483 | 21.643 | 4.193 | 1.00 46.52 |
| MOTA | 18098 | | PHE | 2719 | 43.257 | 21.124 | 6.628 | 1.00 46.28 |
| MOTA | 18099 | CE2 | PHE | 2719 | 44.984 | 20.644 | 5.024 | 1.00 46.72 |
| MOTA | 18100 | CZ | PHE | 2719 | 44.369 | 20.383 | 6.245 | |
| MOTA | 18101 | C | PHE | 271 9 | 42.788 | 25.375 | 5.318 | 1.00 44.37 |
| ATOM | 18102 | 0 | PHE | 2719 | 43.406 | 25.307 | 6.381 | 1.00 43.11 |
| ATOM | 18103 | N | ALA | 2720 | 41.561 | 25.879 | 5.223 | 1.00 42.30 |
| ATOM | 18104 | CA | ALA | 2720 | 40.848 | 26.403 | 6.381 | 1.00 41.78 |
| ATOM | 18105 | CB | ALA | 2720 | 40.263 | 27.772 | 6.049 | 1.00 41.45 |
| ATOM | 18106 | C | ALA | 2720 | 39.738 | 25.467 | 6.860 | 1.00 40.79 |
| ATOM | 18107 | ō | ALA | 2720 | 39.120 | 24.756 | 6.065 | 1.00 39.99 |
| ATOM | 18108 | N | THR | 2721 | 39.495 | 25.481 | 8.169 | 1.00 40.42 |
| ATOM | 18109 | CA | THR | 2721 | 38.459 | 24.659 | 8.797 | 1.00 38.92 |
| | | | | | | | | |
| ATOM | 18110 | CB | THR | 2721 | 39.074 | 23.502 | 9.607 8.787 | 1.00 39.08 |
| MOTA | 18111 | OG1 | | 2721 | | 22.786 | | 1.00 41.05 |
| ATOM | 18112 | CG2 | THR | 2721 | 37.986 | 22.545 | 10.073 | 1.00 41.39 |
| ATOM | 18113 | | THR | 2721 | 37.660 | 25.543 | 9.757 | 1.00 37.36 |
| ATOM | 18114 | 0 | THR | 2721 | 38.181 | 26.531 | 10.269 | 1.00 37.24 |
| MOTA | 18115 | N | ILE | 2722 | 36.404 | 25.188 | 10.010 | 1.00 34.57 |
| MOTA | 18116 | CA | ILE | 2722 | 35.575 | 25.983 | 10.907 | 1.00 33.33 |
| MOTA | 18117 | CB | ILE | 2722 | 34.856 | 27.114 | 10.121 | 1.00 33.46 |
| ATOM | 18118 | CG2 | ILE | 2722 | 33.767 | 26.519 | 9.232 | 1.00 32.91 |
| ATOM | 18119 | CG1 | ILE | 2722 | 34.256 | 28.136 | 11.091 | 1.00 33.34 |
| ATOM | 18120 | CD1 | | 2722 | 33.727 | 29.396 | 10.411 | 1.00 33.25 |
| ATOM | 18121 | C | ILE | 2722 | 34.539 | 25.121 | 11.633 | 1.00 33.03 |
| ATOM | 18122 | ō | ILE | 2722 | 34.165 | 24.048 | | 1.00 32.21 |
| ATOM | 18123 | N | THR | 2723 | 34.089 | 25.591 | 12.791 | 1.00 31.25 |
| | | | | | 51.005 | | | |

| ATOM | 18124 | CA | THR | 2723 | 33.099 | 24.861 | 13.563 | 1.00 30.50 |
|------|---------|-----|-------|------|--------|--------|--------|------------|
| MOTA | 18125 | CB | THR | 2723 | 33.120 | 25.275 | 15.044 | 1.00 31.78 |
| ATOM | 18126 | OG1 | THR | 2723 | 32.810 | 26.669 | 15.150 | 1.00 33.34 |
| ATOM | 18127 | CG2 | THR | 2723 | 34.489 | 25.014 | 15.648 | 1.00 31.14 |
| ATOM | 18128 | C | THR | 2723 | 31.716 | 25.143 | 12.996 | 1.00 29.87 |
| ATOM | 18129 | ō | THR | 2723 | 31.491 | 26.174 | 12.360 | 1.00 29.14 |
| ATOM | 18130 | N | ALA | 2724 | 30.794 | 24.214 | 13.218 | 1.00 27.82 |
| | | | | | 29.428 | 24.214 | 12.739 | 1.00 27.32 |
| ATOM | 18131 | CA | ALA | 2724 | | | | |
| ATOM | 18132 | СВ | ALA | 2724 | 29.332 | 23.966 | 11.271 | 1.00 26.45 |
| ATOM | 18133 | С | ALA | 2724 | 28.556 | 23.462 | 13.594 | 1.00 26.25 |
| MOTA | 18134 | Ο. | ALA | 2724 | 28.991 | 22.388 | 13.999 | 1.00 24.53 |
| MOTA | 18135 | N | TYR | 2725 | 27.336 | 23.905 | 13.877 | 1.00 25.34 |
| ATOM | 18136 | CA | TYR | 2725 | 26.422 | 23.126 | 14.702 | 1.00 25.41 |
| ATOM | 18137 | CB | TYR | 2725 | 26.441 | 23.634 | 16.145 | 1.00 25.02 |
| ATOM | 18138 | CG | TYR | 2725 | 27.818 | 23.940 | 16.681 | 1.00 25.72 |
| ATOM | 18139 | CD1 | TYR | 2725 | 28.264 | 25.257 | 16.791 | 1.00 27.23 |
| ATOM | 18140 | CE1 | TYR | 2725 | 29.534 | 25.548 | 17.278 | 1.00 27.51 |
| ATOM | 18141 | CD2 | TYR | 2725 | 28.678 | 22.916 | 17.071 | 1.00 24.40 |
| ATOM | 18142 | CE2 | TYR | 2725 | 29.951 | 23.195 | 17.557 | 1.00 27.21 |
| | | | | 2725 | 30.372 | 24.515 | 17.659 | 1.00 27.21 |
| ATOM | 18143 | CZ | TYR | | | | | |
| ATOM | 18144 | ОН | TYR | 2725 | 31.632 | 24.797 | 18.149 | 1.00 29.59 |
| MOTA | 18145 | С | TYR | 2725 | 24.996 | 23.188 | 14.181 | 1.00 25.48 |
| ATOM | 18146 | 0 | TYR | 2725 | 24.073 | 22.716 | 14.847 | 1.00 25.90 |
| MOTA | 18147 | N | ASP | 2726 | 24.812 | 23.773 | 12.999 | 1.00 24.99 |
| MOTA | 18148 | CA | ASP | 2726 | 23.475 | 23.895 | 12.424 | 1.00 25.25 |
| MOTA | 18149 | CB | ASP | 2726 | 22.736 | 25.085 | 13.049 | 1.00 24.48 |
| MOTA | 18150 | CG | ASP | 2726 | 23.368 | 26.424 | 12.701 | 1.00 27.30 |
| ATOM | 18151 | OD1 | ASP . | 2726 | 23.278 | 26.844 | 11.529 | 1.00 27.92 |
| ATOM | 18152 | OD2 | ASP | 2726 | 23.954 | 27.055 | 13.608 | 1.00 26.94 |
| ATOM | 18153 | C | ASP | 2726 | 23.463 | 24.023 | 10.906 | 1.00 25.69 |
| ATOM | 18154 | 0 | ASP | 2726 | 24.482 | 24.317 | 10.282 | 1.00 25.88 |
| | 18155 | N | TYR | 2727 | 22.289 | 23.792 | 10.329 | 1.00 25.18 |
| ATOM | | | | | | | 8.890 | |
| ATOM | 18156 | CA | TYR | 2727 | 22.080 | 23.855 | | |
| MOTA | 18157 | CB | TYR | 2727 | 20.607 | 23.601 | 8.575 | 1.00 29.33 |
| MOTA | 18158 | CG | TYR | 2727 | 20.215 | 23.942 | 7.156 | 1.00 32.36 |
| MOTA | 18159 | CD1 | TYR | 2727 | 20.418 | 23.035 | 6.117 | 1.00 33.43 |
| MOTA | 18160 - | CE1 | TYR | 2727 | 20.049 | 23.348 | 4.808 | 1.00 35.74 |
| MOTA | 18161 | CD2 | TYR | 2727 | 19.636 | 25.177 | 6.853 | 1.00 32.74 |
| ATOM | 18162 | CE2 | TYR | 2727 | 19.266 | 25.501 | 5.550 | 1.00 34.63 |
| MOTA | 18163 | CZ | TYR | 2727 | 19.473 | 24.581 | 4.535 | 1.00 34.95 |
| ATOM | 18164 | ОН | TYR | 2727 | 19.090 | 24.890 | 3.250 | 1.00 36.38 |
| ATOM | 18165 | С | TYR | 2727 | 22.481 | 25.185 | 8.261 | 1.00 28.49 |
| ATOM | 18166 | Ō | TYR | 2727 | 23.244 | 25.219 | 7.296 | 1.00 26.62 |
| MOTA | 18167 | N | SER | 2728 | 21.940 | 26.273 | 8.798 | 1.00 29.50 |
| | 18168 | | SER | 2728 | 22.215 | 27.601 | 8.270 | 1.00 25.30 |
| ATOM | | CA | | | | | | |
| MOTA | 18169 | CB | SER | 2728 | 21.606 | 28.670 | 9.174 | 1.00 30.32 |
| MOTA | 18170 | OG | SER | 2728 | 20.195 | 28.606 | 9.127 | 1.00 30.03 |
| MOTA | 18171 | С | SER | 2728 | 23.691 | 27.885 | 8.063 | 1.00 32.53 |
| MOTA | 18172 | 0 | SER | 2728 | 24.151 | 28.017 | 6.927 | 1.00 34.08 |
| MOTA | 18173 | N · | PHE | 2729 | 24.441 | 27.979 | 9.152 | 1.00 33.01 |
| ATOM | 18174 | CA | PHE | 2729 | 25.860 | 28.263 | 9.026 | 1.00 34.03 |
| ATOM | 18175 | CB | PHE | 2729 | 26.514 | 28.379 | 10.402 | 1.00 32.92 |
| ATOM | 18176 | CG | PHE | 2729 | 26.244 | 29.689 | 11.084 | 1.00 33.06 |
| ATOM | 18177 | CD1 | PHE | 2729 | 25.190 | 29.824 | 11.979 | 1.00 32.75 |
| ATOM | 18178 | CD2 | PHE | 2729 | 27.041 | 30.800 | 10.816 | 1.00 33.37 |
| ATOM | 18179 | CE1 | | 2729 | 24.934 | 31.046 | 12.601 | 1.00 33.58 |
| ATOM | 18180 | CE2 | | 2729 | 26.793 | 32.024 | 11.430 | 1.00 33.46 |
| ATOM | 18181 | CZ | PHE | 2729 | 25.738 | 32.148 | 12.325 | 1.00 33.47 |
| ATOM | 18182 | C | PHE | 2729 | 26.598 | 27.241 | 8.171 | 1.00 34.90 |
| | 18183 | | PHE | | 27.417 | 27.614 | 7.333 | 1.00 35.39 |
| ATOM | | 0 | | 2729 | 26.310 | 25.958 | | 1.00 33.39 |
| ATOM | 18184 | N | ALA | 2730 | | | 8.367 | |
| MOTA | 18185 | CA | ALA | 2730 | 26.968 | 24.919 | 7.582 | 1.00 34.81 |
| ATOM | 18186 | CB | ALA | 2730 | 26.409 | 23.544 | 7.949 | 1.00 34.81 |
| ATOM | 18187 | С | ALA | 2730 | 26.744 | 25.198 | 6.099 | 1.00 34.77 |
| ATOM | 18188 | 0 | ALA | 2730 | 27.638 | 25.002 | 5.275 | 1.00 34.75 |
| ATOM | 18189 | N | LYS | 2731 | 25.540 | 25.659 | 5.777 | 1.00 35.58 |
| MOTA | 18190 | CA | LYS | 2731 | 25.154 | 25.983 | 4.408 | 1.00 36.11 |
| ATOM | 18191 | CB | LYS | 2731 | 23.657 | 26.294 | 4.361 | 1.00 37.50 |
| ATOM | 18192 | CG | LYS | 2731 | 23.151 | 26.818 | 3.033 | 1.00 38.67 |
| ATOM | 18193 | CD | LYS | 2731 | 23.122 | 25.740 | 1.977 | 1.00 40.61 |
| ATOM | 18194 | CE | LYS | 2731 | 22.524 | 26.278 | 0.685 | 1.00 42.74 |
| ATOM | 18195 | NZ | LYS | 2731 | 22.418 | 25.227 | -0.361 | 1.00 43.93 |
| ATOM | 18196 | C | LYS | 2731 | 25.938 | 27.189 | 3.909 | 1.00 36.82 |
| | | | | | 26.426 | | 2.777 | 1.00 36.82 |
| ATOM | 18197 | 0 | LYS | 2731 | | 27.204 | | |
| MOTA | 18198 | N | LEU | 2732 | 26.048 | 28.198 | 4.766 | 1.00 37.43 |
| ATOM | 18199 | CA | LEU | 2732 | 26.762 | 29.421 | 4.434 | 1.00 38.34 |
| ATOM | 18200 | CB | LEU | 2732 | 26.576 | 30.449 | 5.558 | 1.00 38.63 |

| | ATOM | 18201 | CG | LEU | 2732 | 27.150 | 31.858 | 5.367 | 1.00 38.74 |
|---|------|--------|-----|-----|------------|--------|--------|--------|------------|
| | ATOM | 18202 | CD1 | | 2732 | 26.427 | 32.832 | 6.281 | 1.00 37.58 |
| | | 18203 | CD2 | | 2732 | 28.643 | 31.853 | 5.652 | 1.00 38.30 |
| | ATOM | | | | | 28.247 | 29.163 | 4.179 | 1.00 38.90 |
| | MOTA | 18204 | C | LEU | 2732 | | | | |
| | MOTA | 18205 | 0 | LEU | 2732 | 28.830 | 29.742 | 3.264 | 1.00 39.61 |
| | MOTA | 18206 | N | PHE | 2733 | 28.861 | 28.292 | 4.976 | 1.00 38.38 |
| | MOTA | 18207 | CA | PHE | 2733 | 30.278 | 27.992 | 4.793 | 1.00 39.32 |
| | MOTA | 18208 | CB | PHE | 2733 | 30.828 | 27.199 | 5.984 | 1.00 38.73 |
| | MOTA | 18209 | CG | PHE | 2733 | 30.623 | 27.870 | 7.314 | 1.00 38.08 |
| | MOTA | 18210 | CD1 | PHE | 2733 | 30.813 | 29.241 | 7.459 | 1.00 37.35 |
| | MOTA | 18211 | CD2 | PHE | 2733 | 30.267 | 27.123 | 8.430 | 1.00 36.25 |
| | MOTA | 18212 | | PHE | 2733 | 30.652 | 29.856 | 8.698 | 1.00 36.41 |
| | ATOM | 18213 | | PHE | 2733 | 30.104 | 27.729 | 9.671 | 1.00 36.51 |
| | ATOM | 18214 | CZ | PHE | 2733 | 30.297 | 29.098 | 9.804 | 1.00 36.45 |
| | | 18215 | C | PHE | 2733 | 30.509 | 27.192 | 3.514 | 1.00 39.89 |
| | MOTA | | | | | | | 2.764 | 1.00 39.04 |
| | ATOM | 18216 | 0 | PHE | 2733 | 31.449 | 27.455 | | 1.00 40.69 |
| | MOTA | 18217 | N | ALA | 2734 | 29.642 | 26.213 | 3.274 | |
| | ATOM | 18218 | CA | ALA | 2734 | 29.746 | 25.366 | 2.094 | 1.00 42.63 |
| | MOTA | 18219 | CB | ALA | 2734 | 28.712 | 24.246 | 2.166 | 1.00 41.54 |
| | MOTA | 18220 | C | ALA | 2734 | 29.564 | 26.157 | 0.800 | 1.00 44.13 |
| | ATOM | 18221 | 0 | ALA | 2734 | 30.273 | 25.926 | -0.177 | 1.00 44.26 |
| | MOTA | 18222 | N | ASP | 2735 | 28.612 | 27.085 | 0.795 | 1.00 45.42 |
| | ATOM | 18223 | CA | ASP | 2735 | 28.354 | 27.889 | -0.394 | 1.00 47.29 |
| | ATOM | 18224 | СВ | ASP | 2735 | 27.145 | 28.802 | -0.185 | 1.00 47.94 |
| | ATOM | 18225 | CG | ASP | 2735 | 25.840 | 28.038 | -0.114 | 1.00 49.27 |
| | | 18226 | | ASP | 2735 | 25.710 | 27.008 | -0.815 | 1.00 49.87 |
| | ATOM | | | | | | | 0.630 | 1.00 49.47 |
| | ATOM | 18227 | | ASP | 2735 | 24.937 | 28.478 | | 1.00 47.96 |
| • | ATOM | 18228 | C | ASP | 2735 | 29.555 | 28.738 | -0.794 | |
| | MOTA | 18229 | 0 | ASP | 2735 | 29.759 | 29.013 | -1.976 | 1.00 47.45 |
| | ATOM | 18230 | N | GLU | 2736 | 30.343 | 29.154 | 0.193 | 1.00 48.95 |
| | ATOM | -18231 | CA | GLU | 2736 | 31.520 | 29.976 | -0.062 | 1.00 50.11 |
| | MOTA | 18232 | CB | GLU | 2736 | 31.884 | 30.780 | 1.187 | 1.00 50.79 |
| | MOTA | 18233 | CG | GLU | 2736 | 30.787 | 31.710 | 1.663 | 1.00 51.69 |
| | MOTA | 18234 | CD | GLU | 2736 | 30.351 | 32.690 | 0.594 | 1.00 52.87 |
| | ATOM | 18235 | OE1 | GLU | 2736 | 31.200 | 33.477 | 0.129 | 1.00 54.23 |
| _ | MOTA | 18236 | OE2 | GLU | 2736 | 29.160 | 32.673 | 0.219 | 1.00 52.97 |
| | MOTA | 18237 | C | GLU | 2736 | 32.717 | 29.139 | -0.494 | 1.00 50.56 |
| | ATOM | 18238 | Õ | GLU | 2736 | 33.330 | 29.405 | -1.528 | 1.00 51.77 |
| | ATOM | 18239 | N | GLY | 2737 | 33.051 | 28.127 | 0.299 | 1.00 50.60 |
| | | | CA | GLY | 2737 | 34.181 | 27.281 | -0.044 | 1.00 49.87 |
| | MOTA | 18240 | | | | | | 1.082 | 1.00 49.32 |
| | ATOM | 18241 | C | GLY | 2737 | 34.630 | 26.374 | | |
| | MOTA | 18242 | 0 | GLY | 2737 | 35.293 | 25.367 | 0.839 | 1.00 49.07 |
| | MOTA | 18243 | N | LEU | 2738 | 34.281 | 26.735 | 2.313 | 1.00 49.01 |
| | MOTA | 18244 | CA | LEU | 2738 | 34.646 | 25.936 | 3.475 | 1.00 48.38 |
| | MOTA | 18245 | CB | LEU | 2738 | 34.252 | 26.658 | 4.765 | 1.00 48.66 |
| | MOTA | 18246 | CG | LEU | 2738 | 35.241 | 27.691 | 5.301 | 1.00 47.93 |
| | MOTA | 18247 | CD1 | LEU | 2738 | 34.628 | 28.435 | 6.473 | 1.00 47.98 |
| | MOTA | 18248 | CD2 | LEU | 2738 | 36.523 | 26.992 | 5.726 | 1.00 49.25 |
| | MOTA | 18249 | С | LEU | 2738 | 33.958 | 24.579 | 3.418 | 1.00 47.74 |
| | MOTA | 18250 | 0 | LEU | 2738 | 32.781 | 24.457 | 3.757 | 1.00 48.29 |
| | ATOM | 18251 | N | ASN | 2739 | 34.701 | 23.564 | 2.986 | 1.00 46.36 |
| | ATOM | 18252 | CA | ASN | 2739 | 34.168 | 22.214 | 2.873 | |
| | | | | | 2739 | 34.513 | 21.624 | 1.502 | 1.00 46.52 |
| | MOTA | 18253 | CB | ASN | | | | 0.356 | 1.00 48.47 |
| | MOTA | 18254 | CG | ASN | 2739 | 34.170 | 22.564 | | |
| | MOTA | 18255 | | ASN | 2739 | 33.080 | 23.142 | 0.315 | 1.00 49.82 |
| | MOTA | 18256 | | ASN | 2739 | 35.096 | 22.714 | -0.586 | 1.00 48.29 |
| | MOTA | 18257 | С | ASN | 2739 | 34.733 | 21.319 | 3.975 | 1.00 43.36 |
| | ATOM | 18258 | 0 | ASN | 2739 | 34.751 | 20.097 | 3.850 | 1.00 44.23 |
| | MOTA | 18259 | N | VAL | 2740 | 35.196 | 21.938 | 5.054 | 1.00 40.65 |
| | ATOM | 18260 | CA | VAL | 2740 | 35.753 | 21.200 | 6.179 | 1.00 38.58 |
| | MOTA | 18261 | CB | VAL | 2740 | 37.294 | 21.276 | 6.180 | 1.00 39.42 |
| | MOTA | 18262 | | VAL | 2740 | 37.863 | 20.397 | 7.282 | 1.00 38.41 |
| | ATOM | 18263 | | VAL | 2740 | 37.836 | 20.840 | 4.826 | 1.00 39.41 |
| | ATOM | 18264 | C | VAL | 2740 | 35.206 | 21.797 | 7.472 | 1.00 37.55 |
| | ATOM | 18265 | ō | VAL | 2740 | 35.670 | 22.843 | 7.932 | 1.00 36.45 |
| | | | | | 2741 | 34.213 | 21.128 | 8.052 | 1.00 35.79 |
| | MOTA | 18266 | N | MET | | | | | |
| | MOTA | 18267 | CA | MET | 2741 | 33.586 | 21.605 | 9.280 | 1.00 33.14 |
| | MOTA | 18268 | CB | MET | 2741 | 32.097 | 21.858 | 9.019 | 1.00 33.81 |
| • | MOTA | 18269 | CG | MET | 2741 | 31.862 | 23.092 | 8.157 | 1.00 33.62 |
| | MOTA | 18270 | SD | MET | 2741 | 30.216 | 23.250 | 7.476 | 1.00 35.47 |
| | MOTA | 18271 | CE | MET | 2741 | 30.583 | 23.290 | 5.712 | 1.00 31.93 |
| , | MOTA | 18272 | С | MET | 2741 | 33.781 | 20.666 | 10.466 | 1.00 31.98 |
| | ATOM | 18273 | 0 | MET | 2741 | 33.970 | 19.461 | 10.301 | 1.00 30.77 |
| | ATOM | 18274 | N | LEU | 2742 | 33.737 | 21.228 | 11.666 | 1.00 30.44 |
| | MOTA | 18275 | CA | LEU | 2742 | 33.927 | 20.442 | 12.870 | 1.00 29.16 |
| | MOTA | 18276 | CB | LEU | 2742 | 35.268 | 20.818 | 13.517 | 1.00 31.59 |
| * | ATOM | 18277 | CG | LEU | 2742 | 35.690 | 20.194 | 14.857 | 1.00 34.91 |
| | | | | | -· | 22.000 | | | |
| | | | | | | | | | |

| ATOM | 18278 | CD1 | LEU | 2742 | 34.985 | 20.907 | 15.998 | 1.00 36.28 |
|--------------|----------------|----------|------------|--------------|------------------|------------------|------------------|--------------------------|
| ATOM | 18279 | CD2 | | 2742 | 35.382 | 18.698 | 14.872 | 1.00 35.47 |
| ATOM | 18280 | С | LEU | 2742 | 32.784 | 20.603 | 13.871 | 1.00 28.08 |
| ATOM | 18281 | 0 | LEU | 2742 | 32.471 | 21.710 | 14.315 | 1.00 26.39 |
| ATOM | 18282 | N | VAL | 2743 | 32.154 | 19.479 | 14.205 | 1.00 26.29 |
| ATOM | 18283 | CA | VAL | 2743 | 31.058 | 19.457 | 15.165 | 1.00 24.79 |
| ATOM | 18284 | CB | VAL | 2743 | 29.926 | 18.504 | 14.705 | 1.00 24.91 |
| ATOM | 18285 | CG1 | VAL | 2743 | 28.798 | 18.501 | 15.733 | 1.00 23.46 |
| ATOM | 18286 | CG2 | VAL | 2743 | 29.399 | 18.927 | 13.336 | 1.00 23.03 |
| MOTA | 18287 | С | VAL | 2743 | 31.660 | 18.942 | 16.468 | 1.00 25.50 |
| ATOM | 18288 | 0 | VAL | 2743 | 31.584 | 17.751 | 16.765 | 1.00 24.89 |
| MOTA | 18289 | N | GLY | 2744 | 32.271 | 19.846 | 17.234 | 1.00 25.53 |
| MOTA | 18290 | CA | GLY | 2744 | 32.909 | 19.460 | 18.482 | 1.00 24.69 |
| MOTA | 18291 | С | GLY | 2744 | 32.088 | 19.678 | 19.739 | 1.00 25.51 |
| MOTA | 18292 | 0 | GLY | 2744 | 31.083 | 20.389 | 19.727 | 1.00 23.34 |
| MOTA | 18293 | N | ASP | 2745 | 32.530 | 19.059 | 20.829 | 1.00 26.45 |
| MOTA | 18294 | CA | ASP | 2745 | 31.846 | 19.170 | 22.109 | 1.00 27.04 |
| MOTA | 18295 | CB | ASP | 2745 | 32.468 | 18.218 | 23.136 | 1.00 28.02 |
| MOTA | 18296 | CG | ASP | 2745 | 33.963 | 18.422 | 23.283 | 1.00 31.06 |
| MOTA | 18297 | | ASP | 2745 | 34.442 | 19.544 | 23.010 | 1.00 31.67 |
| MOTA | 18298 | | ASP | 2745 | 34.655 | 17.469 | 23.674 | 1.00 33.16 |
| MOTA | 18299 | С | ASP | 2745 | 31.888 | 20.599 | 22.646 | 1.00 27.84 |
| ATOM | 18300 | 0 | ASP | 2745 | 31.295 | 20.902 | 23.682 | 1.00 26.58 1.00 27.48 |
| ATOM | 18301 | N | SER | 2746 | 32.598 | 21.476 | 21.946 22.368 | 1.00 27.48 |
| MOTA | 18302 | CA | SER | 2746 | 32.675 | 22.864 | 22.300 | 1.00 26.30 |
| MOTA | 18303 | CB | SER | 2746 | 33.541 | 23.670 | 20.064 | 1.00 20.33 |
| ATOM | 18304 | OG | SER | 2746 | 33.076 31.254 | 23.552 23.417 | 22.398 | 1.00 27.45 |
| ATOM | 18305 | C | SER | 2746 | 30.946 | 24.342 | 23.154 | 1.00 27.43 |
| ATOM | 18306 | O N | SER | 2746 2747 | 30.388 | 22.830 | 21.575 | 1.00 25.07 |
| ATOM | 18307 18308 | CA | LEU LEU | 2747 | 28.988 | 23.244 | 21.501 | 1.00 24.80 |
| ATOM | 18309 | CB | LEU | 2747 | 28.220 | 22.325 | 20.539 | 1.00 24.87 |
| ATOM ATOM | 18310 | CG | LEU | 2747 | 28.127 | 20.828 | 20.860 | 1.00 26.63 |
| MOTA | 18311 | | LEU | 2747 | 26.966 | 20.567 | 21.816 | 1.00 25.96 |
| ATOM | 18312 | | LEU | 2747 | 27.912 | 20.050 | 19.564 | 1.00 25.74 |
| ATOM | 18313 | C | LEU | 2747 | 28.343 | 23.215 | 22.887 | 1.00 22.90 |
| ATOM | 18314 | ō | LEU | 2747 | 27.315 | 23.851 | 23.122 | 1.00 22.29 |
| ATOM | 18315 | N | GLY | 2748 | 28.952 | 22.473 | 23.805 | 1.00 22.88 |
| ATOM | 18316 | CA | GLY | 2748 | 28.414 | 22.396 | 25.151 | 1.00 25.99 |
| ATOM | 18317 | С | GLY | 2748 | 28.449 | 23.744 | 25.842 | 1.00 27.51 |
| ATOM | 18318 | 0 | GLY | 2748 | 27.725 | 23.975 | 26.810 | 1.00 27.90 |
| MOTA | 18319 | N | MET | 2749 | 29.291 | 24.641 | 25.342 | 1.00 29.54 |
| MOTA | 18320 | CA | MET | 2749 | 29.411 | 25.970 | 25.930 | 1.00 30.31 |
| ATOM | 18321 | CB | MET | 2749 | 30.884 | 26.294 | 26.194 | 1.00 32.91 |
| MOTA | 18322 | CG | MET | 2749 | 31.546 | 25.370 | 27.208 | 1.00 35.18 |
| MOTA | 18323 | SD | MET | 2749 | 33.294 | 25.754 | 27.464 | 1.00 42.41 |
| MOTA | 18324 | CE | MET | 2749 | 33.162 | 27,152 | 28.569 | 1.00 40.70 |
| ATOM | 18325 | С | MET | 2749 | 28.798 | 27.044 | 25.042 | 1.00 29.17 |
| ATOM | 18326 | 0 | MET | 2749 | 28.003 | 27.863 | 25.500 | 1.00 30.78 |
| MOTA | 18327 | N | THR | 2750 | 29.162 | 27.029 | 23.767 | 1.00 28.64 |
| ATOM | 18328 | CA | THR | 2750 | 28.662 | 28.016 | 22.827 | 1.00 28.34 |
| MOTA | 18329 | CB | THR | 2750 | 29.546 | 28.057 | 21.570 | 1.00 29.53 |
| ATOM | 18330 | | THR | 2750 | 29.124 | 29.130 | 20.718 | 1.00 33.35 |
| MOTA | 18331 | | THR | 2750 | 29.450 | 26.744 27.787 | 20.816 | 1.00 29.90 |
| MOTA | 18332 | С | THR | 2750 | 27.213 26.495 | 28.731 | 22.409 22.073 | 1.00 27.81 1.00 27.33 |
| MOTA | 18333 | 0 | THR | 2750 | 26.779 | 26.533 | 22.425 | 1.00 27.33 |
| MOTA | 18334 | N | VAL VAL | 2751 2751 | 25.411 | 26.220 | 22.033 | 1.00 26.65 |
| ATOM | 18335 18336 | CA CB | VAL | 2751 | 25.380 | 25.004 | 21.076 | 1.00 27.34 |
| MOTA MOTA | 18337 | | VAL | 2751 | 23.945 | 24.661 | 20.717 | 1.00 25.72 |
| MOTA | 18338 | | VAL | 2751 | 26.182 | 25.316 | 19.817 | 1.00 27.61 |
| MOTA | 18339 | C | VAL | 2751 | 24.508 | 25.940 | 23.231 | 1.00 25.59 |
| ATOM | 18340 | o | VAL | 2751 | 23.459 | 26.565 | 23.380 | 1.00 25.62 |
| ATOM | 18341 | N | GLN | 2752 | 24.924 | 25.008 | 24.085 | 1.00 25.08 |
| ATOM | 18342 | CA | GLN | 2752 | 24.140 | 24.633 | 25.261 | 1.00 25.15 |
| MOTA | 18343 | CB | GLN | 2752 | 24.556 | 23.237 | 25.735 | 1.00 25.01 |
| MOTA | 18344 | CG | GLN | 2752 | 24.136 | 22.122 | 24.776 | 1.00 21.90 |
| MOTA | 18345 | CD | GLN | 2752 | 24.763 | 20.776 | 25.103 | 1.00 19.31 |
| ATOM | 18346 | OE1 | | 2752 | 25.425 | 20.616 | 26.126 | 1.00 20.25 |
| MOTA | 18347 | NE2 | | 2752 | 24.563 | 19.802 | 24.223 | 1.00 16.51 |
| MOTA | 18348 | C | GLN | 2752 | 24.248 | 25.637 | 26.406 | 1.00 27.38 |
| MOTA | 18349 | 0 | GLN | 2752 | 23.303 | 25.818 | 27.179 | 1.00 26.43 |
| MOTA | 18350 | N | GLY | 2753 | 25.401 | 26.286 | 26.522 | 1.00 27.57 |
| MOTA | 18351 | CA | GLY | 2753 | 25.577 | 27.273 | 27.574 | 1.00 29.69 |
| MOTA | 18352 | С | GLY | 2753 | 26.144 | 26.765 | 28.886 | 1.00 30.82 |
| MOTA | 18353 | 0 | GLY | 2753 | 25.954 | 27.394 | 29.928 | 1.00 30.56 |
| MOTA | 18354 | N | HIS | 2754 | 26.836 | 25.631 | 28.842 | 1.00 30.11 |

| ATOM | 18355 | CA | HIS | 2754 | 27.4 | 48 2 | 5.063 | 30.036 | 1.00 32.21 |
|------|-------|-----|-----|------|------|-------|-------|--------|------------|
| ATOM | 18356 | CB | HIS | 2754 | 27.6 | | 3.557 | 29.877 | 1.00 33.27 |
| ATOM | 18357 | CG | HIS | 2754 | 26.3 | | 2.794 | 29.763 | 1.00 34.86 |
| MOTA | 18358 | | HIS | 2754 | 25.8 | | 2.052 | 28.751 | 1.00 34.88 |
| ATOM | 18359 | | HIS | 2754 | 25.4 | | 2.735 | 30.783 | 1.00 35.48 |
| | | | | 2754 | 24.4 | | 1.988 | 30.404 | 1.00 35.76 |
| ATOM | 18360 | | HIS | | | | | | 1.00 35.70 |
| MOTA | 18361 | | HIS | 2754 | 24.6 | | 1.562 | 29.175 | |
| MOTA | 18362 | C | HIS | 2754 | 28.8 | | 5.721 | 30.258 | 1.00 33.24 |
| MOTA | 18363 | 0 | HIS | 2754 | 29.3 | | 6.392 | 29.365 | 1.00 31.50 |
| MOTA | 18364 | N | ASP | 2755 | 29.3 | | 5.511 | 31.442 | 1.00 34.08 |
| MOTA | 18365 | CA | ASP | 2755 | 30.6 | 78 2 | 6.084 | 31.795 | 1.00 35.48 |
| MOTA | 18366 | CB | ASP | 2755 | 30.7 | 89 2 | 6.256 | 33.319 | 1.00 38.54 |
| MOTA | 18367 | CG | ASP | 2755 | 30.6 | B7 2 | 4.941 | 34.070 | 1.00 40.66 |
| MOTA | 18368 | OD1 | ASP | 2755 | 31.5 | 98 2 | 4.093 | 33.934 | 1.00 44.22 |
| MOTA | 18369 | OD2 | ASP | 2755 | 29.6 | 94 2 | 4.749 | 34.805 | 1.00 43.84 |
| MOTA | 18370 | С | ASP | 2755 | 31.8 | 41 2 | 5.240 | 31.285 | 1.00 35.23 |
| ATOM | 18371 | 0 | ASP | 2755 | 32.9 | 99 2 | 5.650 | 31.363 | 1.00 36.04 |
| ATOM | 18372 | N | SER | 2756 | 31.5 | | 4.055 | 30.770 | 1.00 33.43 |
| MOTA | 18373 | CA | SER | 2756 | 32.5 | | 3.161 | 30.239 | 1.00 31.37 |
| MOTA | 18374 | CB | SER | 2756 | 33.1 | | 2.252 | 31.339 | 1.00 29.97 |
| MOTA | 18375 | OG | SER | 2756 | 32.1 | | 1.301 | 31.769 | 1.00 28.60 |
| ATOM | 18376 | C | SER | 2756 | 31.9 | | 2.316 | 29.134 | 1.00 30.66 |
| MOTA | 18377 | o | SER | 2756 | 30.7 | | 2.506 | 28.776 | 1.00 29.90 |
| | | | | | 32.7 | | 1.382 | 28.601 | 1.00 20.30 |
| ATOM | 18378 | N | THR | 2757 | | | | | |
| MOTA | 18379 | CA | THR | 2757 | 32.2 | | 0.520 | 27.526 | 1.00 29.72 |
| MOTA | 18380 | CB | THR | 2757 | 33.2 | | 0.404 | 26.415 | 1.00 29.31 |
| MOTA | 18381 | OG1 | THR | 2757 | 34.4 | | 9.832 | 26.957 | 1.00 27.82 |
| MOTA | 18382 | CG2 | THR | 2757 | 33.6 | | 1.773 | 25.831 | 1.00 29.02 |
| MOTA | 18383 | С | THR | 2757 | 31.8 | | 9.109 | 28.009 | 1.00 29.19 |
| MOTA | 18384 | 0 | THR | 2757 | 31.4 | | 8.275 | 27.227 | 1.00 28.12 |
| MOTA | 18385 | N | LEU | 2758 | 32.1 | 07 1 | 8.842 | 29.293 | 1.00 28.20 |
| MOTA | 18386 | CA | LEU | 2758 | 31.8 | 24 1 | 7.519 | 29.849 | 1.00 27.55 |
| MOTA | 18387 | CB | LEU | 2758 | 32.2 | 41 1 | 7.453 | 31.322 | 1.00 28.03 |
| MOTA | 18388 | CG | LEU | 2758 | 33.6 | 89 1 | 7.047 | 31.630 | 1.00 29.70 |
| MOTA | 18389 | CD1 | LEU | 2758 | 34.6 | 58 1 | 8.019 | 30.978 | 1.00 30.55 |
| MOTA | 18390 | CD2 | LEU | 2758 | 33.8 | | 7.011 | 33.135 | 1.00 30.83 |
| MOTA | 18391 | C | LEU | 2758 | 30.3 | | 7.072 | 29.716 | 1.00 26.67 |
| ATOM | 18392 | 0 . | LEU | 2758 | 30.0 | | 5.899 | 29.450 | 1.00 26.40 |
| ATOM | 18393 | N | PRO | 2759 | 29.4 | | 7.993 | 29.908 | 1.00 26.39 |
| MOTA | 18394 | CD | PRO | 2759 | 29.5 | | 9.394 | 30.346 | 1.00 28.12 |
| | 18395 | CA | PRO | 2759 | 27.9 | | 7.626 | 29.795 | 1.00 26.06 |
| MOTA | | | | 2759 | 27.2 | | 8.895 | 30.250 | 1.00 28.18 |
| ATOM | 18396 | CB | PRO | | | | | | |
| ATOM | 18397 | CG | PRO | 2759 | 28.2 | | 9.993 | 29.929 | 1.00 27.99 |
| ATOM | 18398 | С | PRO | 2759 | 27.5 | | 7.161 | 28.401 | 1.00 25.95 |
| ATOM | 18399 | 0 | PRO | 2759 | 26.4 | | 6.557 | 28.244 | 1.00 24.22 |
| MOTA | 18400 | N | VAL | 2760 | 28.3 | | 7.435 | 27.389 | 1.00 24.76 |
| ATOM | 18401 | CA | VAL | 2760 | 28.0 | | 7.037 | 26.022 | 1.00 23.60 |
| ATOM | 18402 | CB | VAL | 2760 | 28.9 | | 7.697 | 24.999 | 1.00 23.62 |
| MOTA | 18403 | CG1 | VAL | 2760 | 28.6 | 13 1 | 7.292 | 23.592 | 1.00 23.23 |
| MOTA | 18404 | CG2 | VAL | 2760 | 28.9 | 49 1 | 9.204 | 25.135 | 1.00 24.42 |
| MOTA | 18405 | С | VAL | 2760 | 28.1 | 20 1 | 5.528 | 25.853 | 1.00 21.28 |
| ATOM | 18406 | 0 | VAL | 2760 | 29.1 | 42 1 | 4.912 | 26.145 | 1.00 21.37 |
| ATOM | 18407 | N | THR | 2761 | 27.0 | 41 1 | 4.914 | 25.381 | 1.00 21.58 |
| MOTA | 18408 | CA | THR | 2761 | 27.0 | 96 13 | 3.475 | 25.205 | 1.00 22.07 |
| MOTA | 18409 | CB | THR | 2761 | 26.0 | 38 1 | 2.765 | 26.109 | 1.00 25.74 |
| MOTA | 18410 | OG1 | THR | 2761 | 25.0 | | 3.706 | 26.540 | 1.00 27.70 |
| ATOM | 18411 | CG2 | THR | 2761 | 26.7 | | 2.205 | 27.362 | 1.00 29.26 |
| ATOM | 18412 | | THR | 2761 | 27.0 | | 3.062 | 23.731 | 1.00 20.47 |
| ATOM | 18413 | ō | THR | 2761 | 26.8 | | 3.907 | 22.851 | 1.00 18.18 |
| ATOM | 18414 | N | VAL | 2762 | 27.1 | | 1.769 | 23.466 | 1.00 17.63 |
| MOTA | 18415 | CA | VAL | 2762 | 27.1 | | 1.268 | 22.102 | 1.00 17.03 |
| | | CB | VAL | 2762 | 27.2 | | 9.724 | 22.092 | 1.00 16.14 |
| MOTA | 18416 | | | | 27.2 | | 9.186 | 20.676 | 1.00 18.56 |
| MOTA | 18417 | | VAL | 2762 | | | | | |
| MOTA | 18418 | CG2 | | 2762 | 28.6 | | 9.330 | 22.709 | 1.00 17.91 |
| MOTA | 18419 | С | VAL | 2762 | 25.8 | | 1.699 | 21.335 | 1.00 17.74 |
| ATOM | 18420 | 0 | VAL | 2762 | 25.9 | | 2.166 | 20.204 | 1.00 20.33 |
| MOTA | 18421 | N | ALA | 2763 | 24.7 | | 1.555 | 21.950 | 1.00 16.50 |
| MOTA | 18422 | CA | ALA | 2763 | 23.4 | | 1.939 | 21.308 | 1.00 16.78 |
| MOTA | 18423 | CB | ALA | 2763 | 22.2 | | 1.727 | 22.274 | 1.00 17.39 |
| MOTA | 18424 | C | ALA | 2763 | 23.4 | | 3.387 | 20.814 | 1.00 16.99 |
| MOTA | 18425 | О | ALA | 2763 | 22.9 | | 3.679 | 19.732 | 1.00 16.49 |
| MOTA | 18426 | N | ASP | 2764 | 24.0 | | 4.289 | 21.607 | 1.00 16.36 |
| MOTA | 18427 | CA | ASP | 2764 | 24.1 | 18 1 | 5.696 | 21.228 | 1.00 17.12 |
| MOTA | 18428 | CB | ASP | 2764 | 24.7 | 19 1 | 6.544 | 22.355 | 1.00 16.73 |
| MOTA | 18429 | CG | ASP | 2764 | 23.8 | | 6.518 | 23.622 | 1.00 18.74 |
| MOTA | 18430 | | ASP | 2764 | 22.6 | | 6.468 | 23.530 | 1.00 17.10 |
| ATOM | 18431 | | ASP | 2764 | 24.4 | | 6.570 | 24.718 | 1.00 18.91 |
| | | | | | | | | | |

| ATOM | 18432 | С | ASP | 2764 | 24.968 | 15.875 | 19.977 | 1.00 16.55 |
|--------------|----------------|----------|------------|--------------|------------------|--------|--------|------------|
| ATOM | 18433 | ō | ASP | 2764 | 24.617 | 16.642 | 19.084 | 1.00 15.59 |
| | | | | | 26.094 | 15.171 | 19.923 | 1.00 17.15 |
| MOTA | 18434 | N | ILE | 2765 | | | | |
| MOTA | 18435 | CA | ILE | 2765 | 26.991 | 15.261 | 18.774 | 1.00 18.11 |
| MOTA | 18436 | CB | ILE | 2765 | 28.270 | 14.399 | 18.985 | 1.00 18.63 |
| ATOM | 18437 | CG2 | ILE | 2765 | 29.151 | 14.452 | 17.740 | 1.00 19.14 |
| ATOM | 18438 | CG1 | ILE | 2765 | 29.057 | 14.901 | 20.207 | 1.00 18.27 |
| | | CD1 | ILE | 2765 | 29.657 | 16.300 | 20.041 | 1.00 20.11 |
| MOTA | 18439 | _ | | | | | | |
| MOTA | 18440 | С | ILE | 2765 | 26.263 | 14.787 | 17.509 | 1.00 18.09 |
| MOTA | 18441 | 0 | ILE | 2765 | 26.328 | 15.432 | 16.461 | 1.00 17.25 |
| ATOM | 18442 | N | ALA | 2766 | 25.563 | 13.661 | 17.615 | 1.00 17.05 |
| ATOM | 18443 | CA | ALA | 2766 | 24.831 | 13.106 | 16.478 | 1.00 16.59 |
| ATOM | 18444 | CB | ALA | 2766 | 24.201 | 11.765 | 16.858 | 1.00 18.04 |
| | | | | | | | | |
| MOTA | 18445 | С | ALA | 2766 | 23.749 | 14.060 | 15.983 | |
| ATOM | 18446 | 0 | ALA | 2766 | 23.486 | 14.167 | 14.778 | 1.00 14.36 |
| MOTA | 18447 | N | TYR | 2767 | 23.099 | 14.737 | 16.921 | 1.00 15.60 |
| ATOM | 18448 | CA | TYR | 2767 | 22.048 | 15.682 | 16.578 | 1.00 17.66 |
| ATOM | 18449 | CB | TYR | 2767 | 21.439 | 16.269 | 17.853 | 1.00 17.15 |
| MOTA | 18450 | CG | TYR | 2767 | 20.432 | 17.370 | 17.611 | 1.00 18.50 |
| | | | | | | | | 1.00 19.60 |
| MOTA | 18451 | CD1 | TYR | 2767 | 19.212 | 17.107 | 16.998 | |
| ATOM | 18452 | CE1 | TYR | 2767 | 18.269 | 18.113 | 16.811 | 1.00 19.55 |
| MOTA | 18453 | CD2 | TYR | 2767 | 20.689 | 18.671 | 18.028 | 1.00 20.43 |
| ATOM | 18454 | CE2 | TYR | 2767 | 19.754 | 19.684 | 17.845 | 1.00 17.99 |
| MOTA | 18455 | CZ | TYR | 2767 | 18.547 | 19.396 | 17.238 | 1.00 20.45 |
| ATOM | 18456 | OH | TYR | 2767 | 17.607 | 20.389 | 17.067 | 1.00 19.83 |
| | | | | | | | | |
| MOTA | 18457 | С | TYR | 2767 | 22.612 | 16.812 | 15.715 | 1.00 18.01 |
| MOTA | 18458 | 0 | TYR | 2767 | 22.130 | 17.075 | 14.614 | 1.00 19.81 |
| MOTA | 18459 | N | HIS | 2768 | 23.639 | 17.482 | 16.220 | 1.00 19.41 |
| ATOM | 18460 | CA | HIS | 2768 | 24.239 | 18.581 | 15.479 | 1.00 18.71 |
| MOTA | 18461 | CB | HIS | 2768 | 25.205 | 19.354 | 16.387 | 1.00 18.01 |
| | | | | | | | | |
| ATOM | 18462 | CG | HIS | 2768 | 24.513 | 20.100 | 17.490 | |
| MOTA | 18463 | | HIS | 2768 | 24.343 | 19.799 | 18.801 | 1.00 20.46 |
| ATOM | 18464 | ND1 | HIS | 2768 | 23.816 | 21.271 | 17.275 | 1.00 19.52 |
| ATOM | 18465 | CE1 | HIS | 2768 | 23.246 | 21.657 | 18.403 | 1.00 19.84 |
| ATOM | 18466 | | HIS | 2768 | 23.549 | 20.782 | 19.344 | 1.00 19.32 |
| ATOM | 18467 | C | HIS | 2768 | 24.929 | 18.102 | 14.199 | 1.00 17.93 |
| | | | | | | | | |
| MOTA | 18468 | 0 | HIS | 2768 | 24.916 | 18.802 | 13.185 | 1.00 17.64 |
| ATOM | 18469 | N | THR | 2769 | 25.508 | 16.904 | 14.234 | 1.00 17.47 |
| ATOM | 18470 | CA | THR | 2769 | 26.183 | 16.352 | 13.064 | 1.00 18.99 |
| MOTA | 18471 | CB | THR | 2769 | 26.810 | 14.970 | 13.381 | 1.00 19.01 |
| ATOM | 18472 | OG1 | | 2769 | 27.915 | 15.147 | 14.269 | 1.00 19.38 |
| ATOM | 18473 | CG2 | | 2769 | 27.295 | 14.277 | 12.109 | 1.00 19.98 |
| | | | | | | | | |
| MOTA | 18474 | С | THR | 2769 | 25.207 | 16.216 | 11.894 | |
| ATOM | 18475 | 0 | THR | 2769 | 25.539 | 16.554 | 10.759 | 1.00 20.75 |
| ATOM | 18476 | N | ALA | 2770 | 24.005 | 15.720 | 12.173 | 1.00 18.34 |
| MOTA | 18477 | CA | ALA | 2770 | 22.997 | 15.563 | 11.137 | 1.00 20.30 |
| MOTA | 18478 | CB | ALA | 2770 | 21.784 | 14.809 | 11.686 | 1.00 19.96 |
| ATOM | 18479 | C | ALA | 2770 | 22.562 | 16.923 | 10.586 | 1.00 19.65 |
| | | | | | | | | 1.00 19.44 |
| ATOM | 18480 | 0 | ALA | 2770 | 22.303 | 17.058 | 9.387 | |
| MOTA | 18481 | N | ALA | 2771 | 22.481 | 17.931 | 11.453 | 1.00 19.52 |
| ATOM | 18482 | CA | ALA | 2771 | 22.083 | 19.265 | 11.010 | 1.00 19.17 |
| ATOM | 18483 | CB | ALA | 2771 | 21.887 | 20.199 | 12.213 | 1.00 18.60 |
| ATOM | 18484 | С | ALA | 2771 | 23.146 | 19.828 | 10.072 | 1.00 19.51 |
| ATOM | 18485 | Ö | ALA | 2771 | 22.833 | 20.325 | 8.993 | 1.00 20.21 |
| | | | | | 24.405 | | | 1.00 20.13 |
| MOTA | 18486 | N | JAV | 2772 | | 19.740 | 10.481 | |
| MOTA | 18487 | CA | VAL | 2772 | 25.498 | 20.238 | 9.653 | 1.00 22.46 |
| ATOM | 18488 | CB | VAL | 2772 | 26.864 | 19.996 | 10.332 | 1.00 22.59 |
| ATOM | 18489 | CG1 | VAL | 2772 | 27.998 | 20.293 | 9.355 | 1.00 22.59 |
| MOTA | 18490 | | VAL | 2772 | 26.983 | 20.869 | 11.575 | 1.00 20.73 |
| ATOM | 18491 | C | VAL | 2772 | 25.485 | 19.544 | 8.291 | 1.00 23.49 |
| | | | | | | | | |
| ATOM | 18492 | 0 | VAL | 2772 | 25.567 | 20.198 | 7.252 | 1.00 23.77 |
| ATOM | 18493 | N | ARG | 2773 | 25.375 | 18.219 | 8,307 | 1.00 23.50 |
| ATOM | 18494 | CA | ARG | 2773 | 25.352 | 17.435 | 7.079 | 1.00 23.91 |
| ATOM | 18495 | CB | ARG | 2773 | 25.182 | 15.949 | 7.402 | 1.00 23.75 |
| MOTA | 18496 | CG | ARG | 2773 | 25.032 | 15.065 | 6.181 | 1.00 24.41 |
| ATOM | 18497 | CD | ARG | 2773 | 26.215 | 15.217 | 5.241 | 1.00 25.43 |
| | | | | | | | | |
| MOTA | 18498 | NE | ARG | 2773 | 27.458 | 14.746 | 5.840 | 1.00 25.65 |
| ATOM | 18499 | CZ | ARG | 2773 | 28.661 | 14.919 | 5.301 | 1.00 27.67 |
| MOTA | 18500 | NH1 | ARG | 2773 | 28.787 | 15.560 | 4.147 | 1.00 27.55 |
| MOTA | 18501 | | ARG | 2773 | 29.742 | 14.449 | 5.912 | 1.00 24.82 |
| ATOM | 18502 | C | ARG | 2773 | 24.260 | 17.873 | 6.107 | 1.00 23.35 |
| ATOM | 18503 | | ARG | 2773 | 24.485 | 17.909 | 4.897 | 1.00 25.70 |
| | | 0 | | | | | | |
| ATOM | 18504 | N | ARG | 2774 | 23.081 | 18.198 | 6.626 | 1.00 23.07 |
| ATOM | 18505 | CA | ARG | 2774 | 21.979 | 18.639 | 5.777 | 1.00 24.60 |
| ATOM | 18506 | CB | ARG | 2774 | 20.698 | 18.814 | 6.597 | 1.00 24.60 |
| | 10500 | | | | 20 152 | 17 527 | 7 017 | |
| ATOM | | | ARG | 2774 | 20.163 | 17.532 | 7.217 | 1.00 25.89 |
| ATOM ATOM | 18507 18508 | CG CD | ARG ARG | 2774 2774 | 20.163 18.759 | 17.732 | 7.780 | 1.00 25.89 |

| ATOM | 18509 | NE | ARG | 2774 | 18 | .237 | 16.502 | 8 | .381 | 1.00 | 26.44 |
|--------------|----------------|----------|------------|--------------|----|--------------|------------------|------|------|------|----------------|
| ATOM | 18510 | CZ | ARG | 2774 | | .464 | 16.116 | | .634 | 1.00 | 27.67 |
| ATOM | 18511 | NH1 | ARG | 2774 | 19 | .203 | 16.862 | 10 | .445 | 1.00 | 26.75 |
| MOTA | 18512 | NH2 | ARG | 2774 | 17 | .953 | 14.976 | | .078 | | 29.16 |
| MOTA | 18513 | С | ARG | 2774 | | .329 | 19.962 | | .107 | | 26.29 |
| MOTA | 18514 | 0 | ARG | 2774 | | .917 | 20.225 | | .975 | | 25.64 |
| MOTA | 18515 | N | GLY | 2775 | | .095 | 20.786 | | .818 | | |
| MOTA | 18516 | CA | GLY | 2775 | | .491 | 22.081 | | .295 | | 29.16 |
| ATOM | 18517 | C | GLY | 2775 | | .688 | 22.025 | | .365 | 1.00 | 30.64 |
| ATOM | 18518 | 0 | GLY | 2775 | | .869 | 22.911 | | .528 | 1.00 | 30.02 30.40 |
| МОТА МОТА | 18519 18520 | N CA | ALA ALA | 2776 2776 | | .506 .694 | 20.802 | | .691 | 1.00 | 32.03 |
| ATOM | 18521 | CB | ALA | 2776 | | .914 | 21.368 | | .403 | | 31.76 |
| ATOM | 18522 | C | ALA | 2776 | | .900 | 19.315 | | .404 | 1.00 | 32.26 |
| ATOM | 18523 | ō | ALA | 2776 | | .754 | 18.670 | | .006 | | 33.25 |
| ATOM | 18524 | N | PRO | 2777 | | .118 | 18.753 | | .470 | | 32.99 |
| MOTA | 18525 | CD | PRO | 2777 | 25 | .068 | 19.418 | 3 1 | .678 | 1.00 | 33.32 |
| MOTA | 18526 | CA | PRO | 2777 | 26 | .215 | 17.335 | 5 2 | .109 | 1.00 | 33.05 |
| MOTA | 18527 | CB | PRO | 2777 | 25 | .007 | 17.135 | 5 1 | .202 | 1.00 | 34.47 |
| MOTA | 18528 | CG | PRO | 2777 | 24 | .886 | 18.461 | | .526 | | 34.66 |
| ATOM | 18529 | С | PRO | 2777 | | .520 | 16.922 | | .435 | 1.00 | 33.57 |
| MOTA | 18530 | 0 | PRO | 2777 | | .824 | 15.734 | | .349 | | 31.96 |
| MOTA | 18531 | N | ASN | 2778 | | .288 | 17.902 | | .966 | | 33.97 |
| MOTA | 18532 | CA | ASN | 2778 | | .555 | 17.625 | | .296 | | 35.27 |
| MOTA | 18533 | СВ | ASN | 2778 | | .619 | 18.366 | | .046 | | 36.46 |
| MOTA | 18534 | CG | ASN | 2778 | | .554 | 17.909 | | .023 | | |
| MOTA | 18535 | | ASN | 2778 | | .532 | 16.752 | | .435 | | 38.91 |
| MOTA | 18536 | | ASN | 2778 | | .661 | 18.822 | | .399 | | 39.92 |
| ATOM | 18537 | C | ASN | 2778 | | .768 | 18.023 | | .139 | | 34.56 35.51 |
| MOTA | 18538 | 0 | ASN | 2778 | | .884 .558 | 18.090 | | .629 | | 32.91 |
| ATOM ATOM | 18539 18540 | N CA | CYS CYS | 2779 2779 | | .664 | 18.683 | | .285 | | 31.31 |
| ATOM | 18541 | CB | CYS | 2779 | | .202 | 19.708 | | .335 | 1.00 | 32.14 |
| ATOM | 18542 | SG | CYS | 2779 | | .456 | 19.001 | | .868 | | 30.62 |
| ATOM | 18543 | C | CYS | 2779 | | .287 | 17.497 | | .006 | 1.00 | 31.79 |
| ATOM | 18544 | ō | CYS | 2779 | | .665 | 16.444 | | .151 | | 31.60 |
| ATOM | 18545 | N | LEU | 2780 | | .531 | 17.673 | | .436 | | 30.11 |
| ATOM | 18546 | CA | LEU | 2780 | | .231 | 16.647 | | .191 | 1.00 | 29.59 |
| ATOM | 18547 | CB | LEU | 2780 | 35 | .744 | 16.787 | 7 5 | .018 | 1.00 | 29.72 |
| MOTA | 18548 | .CG | LEU | 2780 | 36 | .593 | 15.754 | 5 | .768 | 1.00 | 29.00 |
| MOTA | 18549 | CD1 | LEU | 2780 | 36 | .280 | 14.356 | | .241 | | 29.73 |
| MOTA | 18550 | CD2 | LEU | 2780 | | .070 | 16.064 | | .591 | | 30.17 |
| MOTA | 18551 | С | LEU | 2780 | | .841 | 16.958 | | .632 | | |
| MOTA | 18552 | 0 | LEU | 2780 | | .395 | 17.868 | | .245 | | 28.84 |
| ATOM | 18553 | . N | LEU. | | | .883 | 16.204 | | .160 | 1.00 | 27.59 |
| ATOM | 18554 | CA | LEU | 2781 2781 | | .384 | 16.422 | | 509 | | 25.37 24.75 |
| ATOM ATOM | 18555 18556 | CB CG | LEU LEU | 2781 | | .891 .977 | 16.063 16.721 | | .604 | 1.00 | 23.53 |
| ATOM | 18557 | | LEU | 2781 | | .525 | 16.303 | | .359 | | 23.06 |
| ATOM | 18558 | | LEU | 2781 | | .414 | 16.333 | | .994 | 1.00 | 22.38 |
| ATOM | 18559 | C | LEU | 2781 | | .149 | 15.643 | | .584 | | 25.37 |
| ATOM | 18560 | 0 | LEU | 2781 | 33 | .200 | 14.415 | | .563 | | 23.46 |
| ATOM | 18561 | N | LEU | 2782 | | .758 | 16.372 | | .514 | | 26.91 |
| ATOM | 18562 | CA | LEU | 2782 | 34 | .488 | 15.760 | 11 | .617 | 1.00 | 26.65 |
| MOTA | 18563 | CB | LEU | 2782 | 35 | .891 | 16.349 | 11 | .738 | 1.00 | 29.44 |
| ATOM | 18564 | CG | LEU | 2782 | | .940 | 15.866 | | .736 | | 31.77 |
| MOTA | 18565 | | LEU | 2782 | | .836 | 16.642 | | .435 | | 32.73 |
| ATOM | 18566 | | LEU | 2782 | | .316 | 16.046 | | .354 | | 34.44 |
| ATOM | 18567 | С | LEU | 2782 | | .729 | 16.016 | | .913 | | 26.25 |
| ATOM | 18568 | 0 | LEU | 2782 | | .362 | 17.152 | | .208 | | 26.93 |
| ATOM | 18569 | N | ALA | 2783 | | .495 | 14.966 | | .692 | | 25.81 26.30 |
| MOTA | 18570 | CA | ALA | 2783 | | .775 .397 | 15.116 14.481 | | .843 | | 25.81 |
| ATOM ATOM | 18571 18572 | CB C | ALA ALA | 2783 2783 | | .555 | 14.483 | | .096 | | 23.83 |
| ATOM | 18573 | o | ALA | 2783 | | .175 | 13.439 | | .921 | | 23.35 |
| ATOM | 18574 | N | ASP | 2784 | | .532 | 15.112 | | .267 | | 24.55 |
| MOTA | 18575 | CA | ASP | 2784 | | .258 | 14.565 | | .409 | | 24.44 |
| ATOM | 18576 | CB | ASP | 2784 | | .644 | | | .420 | | 29.43 |
| ATOM | 18577 | CG | ASP | 2784 | | .301 | 16.852 | | .787 | | 30.77 |
| ATOM | 18578 | | ASP | 2784 | | .870 | 16.717 | | .687 | | 34.29 |
| ATOM | 18579 | | ASP | 2784 | | .253 | 17.929 | | .416 | 1.00 | 32.28 |
| ATOM | 18580 | С | ASP | 2784 | | .445 | 13.549 | | .184 | | 22.89 |
| ATOM | 18581 | 0 | ASP | 2784 | | .213 | 13.581 | | .176 | | 22.27 |
| ATOM | 18582 | N | LEU | 2785 | | .151 | 12.641 | | .843 | | 22.16 |
| MOTA | 18583 | CA | LEU | 2785 | | .506 | 11.683 | | .718 | | 21.83 |
| MOTA | 18584 | CB | LEU | 2785 | | .278 | 10.367 | | .788 | | 21.35 |
| ATOM | 18585 | CG | LEU | 2785 | 34 | .145 | 9.458 | 3 19 | .559 | 1.00 | 21.98 |

| ATOM | 18586 | CD1 | LEU | 2785 | | 34.687 | 8.077 | 19.896 | 1.00 22.46 |
|--------------|----------------|-----------|------------|--------------|---|------------------|------------------|--------|------------|
| | 18587 | CD2 | LEU | 2785 | | 32.680 | 9.356 | 19.147 | 1.00 22.46 |
| MOTA | 18588 | С | LEU | 2785 | | 33.629 | 12.440 | 22.032 | 1.00 23.06 |
| MOTA | 18589 | 0 | LEU | 2785 | | 34.738 | 12.760 | 22.472 | 1.00 25.15 |
| ATOM | 18590 | N | PRO | 2786 | | 32.495 | 12.771 | 22.658 | 1.00 22.63 |
| ATOM | 18591 | CD | PRO | 2786 | | 31.134 | 12.348 | 22.285 | 1.00 22.73 |
| ATOM | 18592 | CA | PRO | 2786 | | 32.483 | 13.509 | 23.925 | 1.00 22.23 |
| ATOM | 18593 | СВ | PRO | 2786 | | 30.993 | 13.690 | 24.200 | 1.00 22.61 |
| ATOM | 18594 | CG | PRO | 2786 | | 30.400 | 12.444 | 23.604 | 1.00 24.03 |
| ATOM | 18595 | C | PRO | 2786 | | 33.201 | 12.840 | 25.084 | 1.00 22.35 |
| ATOM | 18596 | 0 | PRO | 2786 | | 33.774 | 11.761 | 24.945 | 1.00 23.47 |
| ATOM | 18597 | N | PHE | 2787 | | 33.157 | 13.511 | 26.232 | 1.00 23.08 |
| ATOM | 18598 | CA | PHE | 2787 | | 33.771 | 13.036 | 27.464 | 1.00 21.93 |
| ATOM | 18599 | CB | PHE | 2787 | | 33.378 | 13.979 | 28.609 | 1.00 24.24 |
| ATOM | 18600 | CG | PHE | 2787 | | 33.721 | 13.461 | 29.974 | 1.00 25.46 |
| ATOM | 18601 | CD1 | | 2787 | | 35.047 | 13.282 | 30.355 | 1.00 28.52 |
| ATOM | 18602 | CD2 | PHE | 2787 | , | 32.714 | 13.151 | 30.885 | 1.00 29.32 |
| ATOM | 18603 | CE1 | PHE | 2787 | | 35.368 | 12.802 | 31.624 | 1.00 29.53 |
| ATOM | 18604 | CE2 | PHE | 2787 | | 33.023 | 12.671 | 32.157 | 1.00 30.35 |
| MOTA | 18605 | CZ | PHE | 2787 | | 34.356 | 12.496 | 32.529 | 1.00 31.34 |
| MOTA | 18606 | C | PHE | 2787 | | 33.359 | 11.598 | 27.800 | 1.00 20.61 |
| ATOM | 18607 | ō | PHE | 2787 | | 32.174 | 11.260 | 27.788 | 1.00 21.01 |
| ATOM | 18608 | N | MET | 2788 | | 34.354 | 10.766 | 28.091 | 1.00 17.86 |
| ATOM | 18609 | CA | MET | 2788 | | 34.156 | 9.364 | 28.452 | 1.00 20.41 |
| ATOM | 18610 | CB | MET | 2788 | | 33.417 | 9.269 | 29.793 | 1.00 21.52 |
| MOTA | 18611 | CG | MET | 2788 | | 33.645 | 7.961 | 30.546 | 1.00 24.11 |
| ATOM | 18612 | SD | MET | 2788 | | 35.397 | 7.699 | 30.917 | 1.00 25.02 |
| | 18613 | CE | MET | 2788 | | 35.761 | 9.174 | 31.844 | 1.00 27.40 |
| MOTA | 18614 | CE | MET | 2788 | | 33.405 | 8.555 | 27.396 | 1.00 19.70 |
| ATOM ATOM | 18615 | 0 | MET | 2788 | | 32.811 | 7.516 | 27.705 | 1.00 22.61 |
| ATOM | 18616 | N | ALA | 2789 | | 33.430 | 9.020 | 26.152 | 1.00 19.87 |
| | 18617 | CA | ALA | 2789 | | 32.736 | 8.321 | 25.069 | 1.00 18.87 |
| MOTA | 18618 | CB | ALA | 2789 | | 32.236 | 9.326 | 24.036 | 1.00 19.03 |
| | 18619 | C | ALA | 2789 | | 33.627 | 7.287 | 24.400 | 1.00 19.61 |
| ATOM | 18620 | 0 | ALA | 2789 | | 33.190 | 6.566 | 23.502 | 1.00 18.35 |
| MOTA | 18621 | N | TYR | 2790 | | 34.880 | 7.213 | 24.832 | 1.00 19.23 |
| MOTA | 18622 | CA | TYR | 2790 | | 35.813 | 6.250 | 24.257 | 1.00 20.39 |
| MOTA | 18623 | CB | TYR | 2790 | | 36.632 | 6.911 | 23.146 | 1.00 21.61 |
| MOTA | | CG | TYR | 2790 | | 37.208 | 8.255 | 23.518 | 1.00 21.98 |
| ATOM | 18624 18625 | | TYR | 2790 | | 38.509 | 8.373 | 24.012 | 1.00 24.51 |
| ATOM | 18626 | CE1 | | 2790 | | 39.039 | 9.625 | 24.362 | 1.00 26.09 |
| ATOM | | CD2 | TYR | 2790 | | 36.445 | 9.413 | 23.385 | 1.00 22.55 |
| MOTA | 18627 18628 | CE2 | TYR | 2790 | | 36.958 | 10.661 | 23.731 | 1.00 25.20 |
| MOTA | | CZ | TYR | 2790 | | 38.252 | 10.760 | 24.216 | 1.00 26.07 |
| ATOM | 18629 | OH | TYR | 2790 | | 38.752 | 12.006 | 24.538 | 1.00 28.26 |
| ATOM | 18630 | C | TYR | 2790 | | 36.720 | 5.685 | 25.331 | 1.00 21.20 |
| MOTA | 18631 18632 | 0 | TYR | 2790 | | 37.905 | 5.452 | 25.099 | 1.00 20.79 |
| ATOM | 18633 | N | ALA | 2791 | | 36.136 | 5.443 | 26.501 | 1.00 20.62 |
| ATOM | | | ALA | 2791 | | 36.863 | 4.902 | 27.649 | 1.00 22.09 |
| ATOM | 18634 18635 | CA CB | ALA. | 2791 | | 35.957 | 4.894 | 28.876 | 1.00 23.98 |
| ATOM | | CB | ALA | 2791 | | 37.401 | 3.496 | 27.383 | 1.00 21.97 |
| ATOM | 18636 | | | 2791 | | 38.381 | 3.075 | 27.994 | 1.00 22.52 |
| ATOM | 18637 | 0 | ALA THR | 2792 | | 36.740 | 2.766 | 26.491 | 1.00 20.00 |
| MOTA | 18638 | N | THR | 2792 | | 37.186 | 1.431 | 26.123 | 1.00 20.70 |
| MOTA | 18639 18640 | CA CB | THR | 2792 | | 36.348 | 0.313 | 26.786 | 1.00 21.59 |
| MOTA | 18641 | OG1 | | 2792 | | 35.030 | 0.310 | 26.220 | 1.00 23.40 |
| ATOM ATOM | 18642 | CG2 | | 2792 | | 36.250 | 0.532 | 28.297 | 1.00 20.98 |
| | | CG2 | THR | 2792 | | 36.999 | 1.325 | 24.616 | 1.00 21.35 |
| MOTA | 18643 | 0 | THR | 2792 | | 36.128 | 1.980 | 24.052 | 1.00 19.07 |
| MOTA | 18644 18645 | N | PRO | 2793 | | 37.824 | 0.510 | 23.945 | 1.00 21.50 |
| ATOM | | | PRO | 2793 | | 38.961 | -0.267 | 24.471 | 1.00 22.59 |
| MOTA | 18646 18647 | CD CA | PRO | 2793 | | 37.711 | 0.348 | 22.494 | 1.00 22.71 |
| MOTA | | | | 2793 | | 38.738 | -0.737 | 22.197 | 1.00 23.86 |
| ATOM | 18648 | CB | PRO | 2793 | | 39.806 | -0.458 | 23.233 | 1.00 24.23 |
| ATOM | 18649 | CG | PRO | 2793 | | 36.290 | -0.458 | 22.097 | 1.00 24.23 |
| ATOM | 18650 | С | PRO | | | 35.740 | 0.462 | 21.124 | 1.00 21.75 |
| ATOM | 18651 | O N | PRO | 2793 2794 | | 35.694 | -0.954 | 22.867 | 1.00 20.31 |
| MOTA | 18652 | N | GLU | 2794 | | 34.341 | -1.412 | 22.588 | 1.00 22.74 |
| MOTA | 18653 | CA | GLU | | | 33.932 | -2.482 | 23.603 | 1.00 22.74 |
| ATOM | 18654 | CB | GLU | 2794 | | 33.932 | -3.362 | 23.157 | 1.00 20.70 |
| ATOM | 18655 | CG | GLU | 2794 2794 | | 32.776 | -4.484 | 24.143 | 1.00 32.07 |
| ATOM | 18656 | CD OF1 | GLU | | | | -4.484 -4.182 | 25.291 | 1.00 37.20 |
| MOTA | 18657 | OE1 | | 2794 | | 32.076 | -4.182 -5.669 | 23.771 | 1.00 38.38 |
| MOTA | 18658 | OE2 | | 2794 | | 32.659 | -0.231 | 22.628 | 1.00 39.39 |
| ATOM | 18659 | С | GLU | 2794 | | 33.367 32.536 | -0.231 | 21.734 | 1.00 21.49 |
| ATOM | 18660 | O N | GLU | 2794 | | 32.536 | 0.609 | 23.652 | 1.00 18.00 |
| MOTA | 18661 | . N | GLN | 2795 | | | 1.758 | 23.728 | 1.00 19.70 |
| MOTA | 18662 | CA | GLN | 2795 | | 32.574 | 1.756 | 23.120 | 1.00 13.37 |

| MOTA | 18663 | CB | GLN | 2795 | 32.708 | 2.444 | 25.086 | 1.00 23.38 |
|--------------|----------------|----------|------------|--------------|------------------|-----------------|------------------|--------------------------|
| MOTA | 18664 | CG | GLN | 2795 | 32.276 | 1.563 | 26.239 | 1.00 30.06 |
| MOTA | 18665 | CD | GLN | 2795 | 32.302 | 2.296 | 27.555 | 1.00 33.76 |
| MOTA | 18666 | | GLN | 2795 | 31.557 | 3.257 | 27.755 | 1.00 37.23 |
| MOTA | 18667 | | GLN GLN | 2795 2795 | 33.164 32.883 | 1.854 2.738 | 28.463 22.602 | 1.00 37.36 1.00 18.75 |
| ATOM ATOM | 18668 18669 | C 0 | GLN | 2795 | 31.979 | 3.379 | 22.055 | 1.00 16.73 |
| ATOM | 18670 | N | ALA | 2796 | 34.160 | 2.853 | 22.251 | 1.00 17.68 |
| MOTA | 18671 | CA | ALA | 2796 | 34.561 | 3.740 | 21.161 | 1.00 16.76 |
| MOTA | 18672 | CB | ALA | 2796 | 36.077 | 3.731 | 21.019 | 1.00 17.78 |
| ATOM | 18673 | С | ALA | 2796 | 33.909 | 3.306 | 19.844 | 1.00 15.71 |
| MOTA | 18674 | 0 | ALA | 2796 | 33.408 | 4.146 | 19.097 | 1.00 13.16 |
| MOTA | 18675 | N | PHE | 2797 2797 | 33.897 33.302 | 2.002 1.508 | 19.567 18.319 | 1.00 16.19 1.00 16.66 |
| ATOM ATOM | 18676 18677 | CA CB | PHE PHE | 2797 | 33.374 | -0.023 | 18.233 | 1.00 15.73 |
| ATOM | 18678 | CG | PHE | 2797 | 34.749 | -0.596 | 18.450 | 1.00 19.24 |
| ATOM | 18679 | | PHE | 2797 | 35.882 | 0.081 | 18.013 | 1.00 17.94 |
| MOTA | 18680 | CD2 | PHE | 2797 | 34.907 | -1.823 | 19.088 | 1.00 17.33 |
| MOTA | 18681 | | PHE | 2797 | 37.153 | -0.453 | 18.212 | 1.00 20.94 |
| ATOM | 18682 | | PHE | 2797 | 36.175 | -2.369 | 19.293 | 1.00 20.14 |
| MOTA | 18683 18684 | CZ | PHE PHE | 2797 2797 | 37.299 31.840 | -1.678 1.925 | 18.853 18.221 | 1.00 18.91 1.00 15.33 |
| MOTA MOTA | 18685 | C O | PHE | 2797 | 31.398 | 2.438 | 17.197 | 1.00 13.33 |
| ATOM | 18686 | N | GLU | 2798 | 31.105 | 1.688 | 19.305 | 1.00 17.31 |
| ATOM | 18687 | CA | GLU | 2798 | 29.687 | 2.015 | 19.392 | 1.00 18.59 |
| ATOM | 18688 | CB | GLU | 2798 | 29.139 | 1.537 | 20.741 | 1.00 23.40 |
| MOTA | 18689 | CG | GLU | 2798 | 27.645 | 1.743 | 20.953 | 1.00 27.48 |
| MOTA | 18690 | CD. | GLU | 2798 | 26.801 | 0.925 | 19.996 | 1.00 31.32 |
| MOTA | 18691 | | GLU | 2798 | 27.266 | -0.155 | 19.566 | 1.00 34.20 |
| MOTA | 18692 | | GLU | 2798 | 25.667 | 1.353 | 19.685 | 1.00 34.45 |
| ATOM | 18693 | C | GLU | 2798 | 29.379 | 3.507 | 19.220 | 1.00 17.82 1.00 16.21 |
| MOTA MOTA | 18694 18695 | O N | GLU ASN | 2798 2799 | 28.510 30.082 | 3.882 4.363 | 18.432 19.956 | 1.00 10.21 |
| ATOM | 18696 | CA | ASN | 2799 | 29.808 | 5.790 | 19.863 | 1.00 16.33 |
| ATOM | 18697 | CB | ASN | 2799 | 30.402 | 6.521 | 21.069 | 1.00 17.15 |
| ATOM | 18698 | CG | ASN | 2799 | 29.710 | 6.125 | 22.369 | 1.00 20.67 |
| ATOM | 18699 | OD1 | ASN | 2799 | 28.495 | 5.923 | 22.388 | 1.00 17.99 |
| MOTA | 18,700 | ND2 | ASN | 2799 | 30.474 | 6.017 | 23.455 | 1.00 17.98 |
| MOTA | 18701 | C | ASN | 2799 | 30.267 | 6.411 | 18.553 | 1.00 15.61 |
| ATOM | 18702 | 0 | ASN | 2799 | 29.615 | 7.313 | 18.031 | 1.00 15.62 |
| ATOM | 18703 18704 | N CA | ALA ALA | 2800 2800 | 31.379 31.891 | 5.915 6.395 | 18.019 16.748 | 1.00 16.20 1.00 16.55 |
| ATOM ATOM | 18704 | CB | ALA | 2800 | 33.233 | 5.752 | 16.443 | 1.00 14.64 |
| ATOM | 18706 | C | ALA | 2800 | 30.885 | 6.050 | 15.653 | 1.00 16.73 |
| ATOM | 18707 | Ō | ALA | 2800 | 30.570 | 6.877 | 14.792 | 1.00 17.09 |
| MOTA | 18708 | N | ALA | 2801 | 30.375 | 4.825 | 15.678 | 1.00 16.50 |
| MOTA | 18709 | CA | ALA | 2801 | 29.413 | 4.412 | 14.663 | 1.00 16.96 |
| MOTA | 18710 | CB | ALA | 2801 | 29.023 | 2.953 | 14.865 | 1.00 17.94 |
| ATOM | 18711 | C | ALA | 2801 | 28.180 | 5.306 | 14.726 | 1.00 15.19 1.00 17.52 |
| ATOM ATOM | 18712 18713 | O N | ALA THR | 2801 2802 | 27.618 27.765 | 5.662 5.679 | 13.696 15.934 | 1.00 17.52 1.00 16.31 |
| ATOM | 18714 | CA | THR | 2802 | 26.596 | 6.528 | 16.082 | 1.00 15.68 |
| ATOM | 18715 | CB | THR | 2802 | 26.265 | 6.808 | 17.572 | 1.00 16.35 |
| ATOM | 18716 | OG1 | | 2802 | 25.995 | 5.577 | 18.252 | 1.00 14.35 |
| MOTA | 18717 | CG2 | THR | 2802 | 25.041 | 7.713 | 17.681 | 1.00 14.96 |
| ATOM | 18718 | С | THR | 2802 | 26.778 | 7.869 | 15.369 | 1.00 16.13 |
| ATOM | 18719 | 0 | THR | 2802 | 25.895 | 8.318 | 14.636 | 1.00 17.22 |
| ATOM ATOM | 18720 18721 | N | VAL VAL | 2803 2803 | 27.921 28.186 | 8.509 9.798 | 15.580 14.956 | 1.00 16.63 1.00 17.54 |
| ATOM | 18721 | CA CB | VAL | 2803 | 29.380 | 10.502 | 15.644 | 1.00 17.34 |
| ATOM | 18723 | | VAL | 2803 | 29.719 | 11.786 | 14.915 | 1.00 23.96 |
| ATOM | 18724 | | VAL | 2803 | 29.023 | 10.813 | 17.098 | 1.00 20.56 |
| MOTA | 18725 | С | VAL | 2803 | 28.449 | 9.669 | 13.458 | 1.00 16.45 |
| MOTA | 18726 | 0 | VAL | 2803 | 28.126 | 10.574 | 12.684 | 1.00 18.21 |
| ATOM | 18727 | N | MET | 2804 | 29.029 | 8.547 | 13.051 | 1.00 16.81 |
| ATOM | 18728 | CA | MET | 2804 | 29.303 | 8.304 | 11.639 | 1.00 17.14 |
| MOTA | 18729 | CB CG | MET MET | 2804 | 30.229 31.654 | 7.093 7.295 | 11.480 11.995 | 1.00 18.19 1.00 22.52 |
| MOTA MOTA | 18730 18731 | SD | MET | 2804 2804 | 32.594 | 8.461 | 10.990 | 1.00 22.32 |
| ATOM | 18732 | CE | MET | 2804 | 32.659 | 7.556 | 9.422 | 1.00 24.27 |
| ATOM | 18733 | C | MET | 2804 | 27.984 | 8.063 | 10.903 | 1.00 16.01 |
| ATOM | 18734 | O | MET | 2804 | 27.761 | 8.618 | 9.824 | 1.00 15.88 |
| ATOM | 18735 | N | ARG | 2805 | 27.101 | 7.248 | 11.481 | 1.00 15.73 |
| MOTA | 18736 | CA | ARG | 2805 | 25.822 | 6.986 | 10.831 | 1.00 15.34 |
| MOTA | 18737 | CB | ARG | 2805 | 25.011 | 5.925 | 11.596 | 1.00 13.01 |
| MOTA MOTA | 18738 18739 | CG | ARG ARG | 2805 | 25.647 24.645 | 4.539 3.460 | 11.632 12.060 | 1.00 16.75 1.00 13.35 |
| AT OF | 10133 | CD | TVG. | 2805 | 24.043 | 2.400 | 12.000 | 1.00 13.33 |

| MOTA | 18740 | NE | ARG | 2805 | 25.314 | 2.212 | 12.432 | 1.00 18.35 |
|--------------|----------------|----------|------------|--------------|------------------|------------------|------------------|--------------------------|
| MOTA | 18741 | CZ | ARG | 2805 | 25.762 | 1.941 | 13.652 | 1.00 16.28 |
| MOTA | 18742 | | ARG | 2805 | 25.609 | 2.829 | 14.630 | 1.00 18.45 |
| MOTA | 18743 | NH2 | ARG | 2805 | 26.369 | 0.789 | 13.894 | 1.00 17.59 |
| MOTA | 18744 | С | ARG | 2805 | 24.999 | 8.268 | 10.718 | 1.00 15.55 |
| ATOM | 18745 | 0 | ARG | 2805 | 24.179 25.232 | 8.404 | 9.817 | 1.00 14.99 1.00 16.80 |
| ATOM | 18746 | N | ALA | 2806 | 25.232 | 9.207 10.473 | 11.633 11.639 | 1.00 16.80 |
| MOTA | 18747 18748 | CA CB | ALA ALA | 2806 2806 | 24.548 | 11.095 | 13.030 | 1.00 16.95 |
| ATOM ATOM | 18749 | C | ALA | 2806 | 24.997 | 11.483 | 10.602 | 1.00 18.90 |
| ATOM | 18750 | ō | ALA | 2806 | 24.425 | 12.567 | 10.466 | 1.00 16.85 |
| ATOM | 18751 | N | GLY | 2807 | 26.062 | 11.144 | 9.880 | 1.00 17.86 |
| MOTA | 18752 | CA | GLY | 2807 | 26.555 | 12.055 | 8.862 | 1.00 20.83 |
| MOTA | 18753 | С | GLY | 2807 | 28.042 | 12.344 | 8.866 | 1.00 19.96 |
| MOTA | 18754 | 0 | GLY | 2807 | 28.583 | 12.841 | 7.873 | 1.00 20.33 |
| MOTA | 18755 | N | ALA | 2808 | 28.706 | 12.039 | 9.976 | 1.00 20.84 |
| ATOM | 18756 | CA | ALA | 2808 | 30.141 | 12.279 | 10.094 | 1.00 20.51 |
| ATOM | 18757 | CB | ALA | 2808 | 30.596 | 12.030 | 11.532 | 1.00 21.43 1.00 22.32 |
| MOTA | 18758 | C | ALA | 2808 2808 | 30.983 30.583 | 11.433 10.340 | 9.140 8.734 | 1.00 22.32 |
| ATOM ATOM | 18759 18760 | N O | ALA ASN | 2809 | 32.154 | 11.954 | 8.783 | 1.00 21.83 |
| ATOM | 18761 | CA | ASN | 2809 | 33.076 | 11.252 | 7.895 | 1.00 23.00 |
| MOTA | 18762 | СВ | ASN | 2809 | 33.563 | 12.161 | 6.756 | 1.00 23.04 |
| ATOM | 18763 | CG | ASN | 2809 | 32.454 | 12.563 | 5.813 | 1.00 22.97 |
| ATOM | 18764 | OD1 | ASN | 2809 | 31.720 | 11.715 | 5.303 | 1.00 26.20 |
| ATOM | 18765 | ND2 | ASN | 2809 | 32.329 | 13.856 | 5.567 | 1.00 24.82 |
| ATOM | 18766 | C | ASN | 2809 | 34.281 | 10.828 | 8.713 | 1.00 23.50 |
| MOTA | 18767 | 0 | ASN | 2809 | 34.991 | 9.885 | 8.365 | 1.00 22.98 |
| ATOM | 18768 | N | MET | 2810 | 34.503 | 11.531 | 9.815 | 1.00 23.62 |
| ATOM | 18769 | CA | MET | 2810 | 35.642 | 11.247 | 10.669 | 1.00 23.93 1.00 25.09 |
| MOTA | 18770 | CB | MET | 2810 | 36.853 38.126 | 12.052 11.879 | 10.181 10.995 | 1.00 24.78 |
| MOTA MOTA | 18771 18772 | CG SD | MET MET | 2810 2810 | 39.481 | 12.847 | 10.255 | 1.00 24.70 |
| ATOM | 18773 | CE | MET | 2810 | 40.353 | 11.582 | 9.303 | 1.00 27.11 |
| ATOM | 18774 | C | MET | 2810 | 35.318 | 11.602 | 12.112 | 1.00 22.92 |
| ATOM | 18775 | 0 | MET | 2810 | 34.490 | 12.469 | 12.377 | 1.00 22.76 |
| ATOM | 18776 | N | VAL | 2811 | 35.972 | 10.912 | 13.037 | 1.00 21.54 |
| MOTA | 18777 | CA | VAL | 2811 | 35.767 | 11.144 | 14.452 | 1.00 22.27 |
| ATOM | 18778 | CB | VAL | 2811 | 35.345 | 9.840 | 15.156 | 1.00 22.64 |
| ATOM | 18779 | | LAV | 2811 | 35.310 | 10.042 | 16.639 | 1.00 27.23 |
| ATOM | 18780 | CG2 | LAV | 2811 | 33.972 | 9.399 11.665 | 14.652 15.092 | 1.00 23.31 1.00 21.34 |
| ATOM | 18781 18782 | С 0 | VAL VAL | 2811 2811 | 37.052 38.151 | 11.238 | 14.729 | 1.00 20.30 |
| ATOM ATOM | 18783 | N | LYS | 2812 | 36.912 | 12.593 | 16.037 | 1.00 21.70 |
| ATOM | 18784 | CA | LYS | 2812 | 38.066 | 13.153 | 16.737 | 1.00 21.55 |
| ATOM | 18785 | CB | LYS | 2812 | 38.114 | 14.679 | 16.577 | 1.00 20.79 |
| ATOM | 18786 | CG | LYS | 2812 | 39.283 | 15.330 | 17.324 | 1.00 22.48 |
| MOTA | 18787 | CD | LYS | 2812 | 39.567 | 16.749 | 16.830 | 1.00 21.07 |
| MOTA | 18788 | CE | LYS | 2812 | 38.508 | 17.730 | 17.295 | 1.00 21.59 |
| MOTA | 18789 | NZ | LYS | 2812 | 38.526 | 17.887 | 18.777 | 1.00 19.95 |
| ATOM | 18790 | C | LYS | 2812 | 38.027 37.000 | 12.803 | 18.216 | 1.00 21.09 1.00 20.83 |
| ATOM | 18791 | O N | LYS | 2812 | 37.000 | 12.967 12.311 | 18.873 18.729 | 1.00 20.83 |
| ATOM ATOM | 18792 18793 | N CA | ILE ILE | 2813 2813 | 39.271 | 11.941 | 20.138 | 1.00 25.12 |
| ATOM | 18794 | CB | ILE | 2813 | 39.341 | 10.403 | 20.318 | 1.00 26.14 |
| ATOM | 18795 | | ILE | 2813 | 38.018 | 9.763 | 19.878 | 1.00 25.11 |
| ATOM | 18796 | | ILE | 2813 | 40.495 | 9.829 | 19.499 | 1.00 27.05 |
| MOTA | 18797 | CD1 | ILE | 2813 | 40.733 | 8.341 | 19.742 | 1.00 28.78 |
| MOTA | 18798 | C | ILE | 2813 | 40.542 | 12.560 | 20.735 | 1.00 27.72 |
| MOTA | 18799 | 0 | ILE | 2813 | 41.580 | 12.607 | 20.078 | 1.00 26.81 |
| MOTA | 18800 | N | GLU | 2814 | 40.454 | 13.028 | 21.978 | 1.00 29.43 |
| MOTA | 18801 | CA | GLU | 2814 | 41.591 | 13.651 | 22.650 | 1.00 32.04 1.00 34.21 |
| ATOM ATOM | 18802 18803 | CB | GLU GLU | 2814 2814 | 41.106 40.144 | 14.813 15.750 | 23.522 22.806 | 1.00 34.21 |
| ATOM | 18804 | CG CD | GLU | 2814 | 39.764 | 16.966 | 23.636 | 1.00 41.47 |
| ATOM | 18805 | | GLU | 2814 | 39.370 | 16.798 | 24.812 | 1.00 41.55 |
| ATOM | 18806 | | GLU | 2814 | 39.852 | 18.093 | 23.105 | 1.00 44.11 |
| MOTA | 18807 | c | GLU | 2814 | 42.364 | 12.655 | 23.509 | 1.00 31.92 |
| ATOM | 18808 | 0 | GLU | 2814 | 41.779 | 11.914 | 24.296 | 1.00 33.22 |
| MOTA | 18809 | N | GLY | 2815 | 43.684 | 12.641 | 23.354 | 1.00 30.77 |
| MOTA | 18810 | CA | GLY | 2815 | 44.506 | 11.729 | 24.126 | 1.00 30.34 |
| ATOM | 18811 | С | GLY | 2815 | 45.801 | 11.392 | 23.415 | 1.00 31.29 |
| ATOM | 18812 | 0 | GLY | 2815 | 45.975 | 11.705 | 22.234 | 1.00 30.87 |
| ATOM ATOM | 18813 18814 | N CA | GLY GLY | 2816 2816 | 46.715 47.992 | 10.748 10.387 | 24.134 23.547 | 1.00 31.99 1.00 33.07 |
| ATOM | 18815 | CA | GLY | 2816 | 47.992 | 8.903 | 23.294 | 1.00 33.07 |
| ATOM | 18816 | ō | GLY | 2816 | 47.325 | 8.261 | 22.675 | 1.00 34.33 |
| | | | | | | | | |

| ATOM | 18817 | N | GLU | 2817 | 49.285 | 8.364 | 23.783 | 1.00 34.03 |
|------|-------|-----|-----|------|--------|--------|--------|------------|
| ATOM | 18818 | CA | GLU | 2817 | 49.631 | 6.956 | 23.615 | 1.00 34.66 |
| ATOM | 18819 | CB | GLU | 2817 | 50.925 | 6.647 | 24.376 | 1.00 37.31 |
| ATOM | 18820 | CG | GLU | 2817 | 52.196 | 7.025 | 23.634 | 1.00 40.46 |
| | | | GLU | 2817 | 52.586 | 5.990 | 22.591 | 1.00 42.88 |
| MOTA | 18821 | CD | | | | | | 1.00 44.37 |
| MOTA | 18822 | OE1 | | 2817 | 51.711 | 5.590 | 21.793 | |
| MOTA | 18823 | OE2 | GLU | 2817 | 53.767 | 5.582 | 22.567 | 1.00 42.78 |
| MOTA | 18824 | С | GLU | 2817 | 48.569 | 5.946 | 24.032 | 1.00 33.69 |
| ATOM | 18825 | 0 | GLU | 2817 | 48.395 | 4.923 | 23.369 | 1.00 34.29 |
| MOTA | 18826 | N | TRP | 2818 | 47.866 | 6.220 | 25.127 | 1.00 32.46 |
| ATOM | 18827 | CA | TRP | 2818 | 46.855 | 5.290 | 25.613 | 1.00 30.43 |
| ATOM | 18828 | СВ | TRP | 2818 | 46.254 | 5.779 | 26.942 | 1.00 30.40 |
| ATOM | 18829 | CG | TRP | 2818 | 45.293 | 6.930 | 26.822 | 1.00 29.06 |
| | | CD2 | TRP | 2818 | 43.862 | 6.850 | 26.831 | 1.00 28.87 |
| MOTA | 18830 | | | | | | | |
| MOTA | 18831 | CE2 | TRP | 2818 | 43.367 | 8.166 | 26.698 | 1.00 28.69 |
| MOTA | 18832 | CE3 | TRP | 2818 | 42.950 | 5.791 | 26.941 | 1.00 27.56 |
| MOTA | 18833 | CD1 | TRP | 2818 | 45.601 | 8.252 | 26.684 | 1.00 30.79 |
| MOTA | 18834 | NE1 | TRP | 2818 | 44.448 | 9.005 | 26.609 | 1.00 30.25 |
| MOTA | 18835 | CZ2 | TRP | 2818 | 41.997 | 8.451 | 26.667 | 1.00 27.27 |
| ATOM | 18836 | CZ3 | TRP | 2818 | 41.590 | 6.074 | 26.910 | 1.00 27.33 |
| ATOM | 18837 | CH2 | TRP | 2818 | 41.127 | 7.399 | 26.776 | 1.00 27.02 |
| ATOM | 18838 | С | TRP | 2818 | 45.737 | 5.048 | 24.604 | 1.00 28.89 |
| MOTA | 18839 | ō | TRP | 2818 | 44.964 | 4.105 | 24.741 | 1.00 30.31 |
| | | N | LEU | 2819 | 45.656 | 5.892 | 23.585 | 1.00 27.35 |
| ATOM | 18840 | | | 2819 | | | 22.579 | 1.00 27.33 |
| MOTA | 18841 | CA | LEU | | 44.616 | 5.744 | | |
| ATOM | 18842 | CB | LEU | 2819 | 44.132 | 7.118 | 22.115 | 1.00 26.77 |
| MOTA | 18843 | CG | LEU | 2819 | 43.245 | 7.896 | 23.085 | 1.00 28.13 |
| ATOM | 18844 | CD1 | LEU | 2819 | 42.926 | 9.257 | 22.487 | 1.00 29.42 |
| MOTA | 18845 | CD2 | LEU | 2819 | 41.969 | 7.121 | 23.358 | 1.00 29.42 |
| MOTA | 18846 | С | LEU | 2819 | 45.040 | 4.930 | 21.364 | 1.00 25.13 |
| ATOM | 18847 | 0 | LEU | 2819 | 44.218 | 4.647 | 20.497 | 1.00 21.39 |
| ATOM | 18848 | N | VAL | 2820 | 46.315 | 4.550 | 21.297 | 1.00 24.43 |
| ATOM | 18849 | CA | VAL | 2820 | 46.814 | 3.783 | 20.155 | 1.00 26.56 |
| | 18850 | CB | VAL | 2820 | 48.258 | 3.281 | 20.395 | 1.00 26.68 |
| ATOM | | | | | | | | |
| ATOM | 18851 | | VAL | 2820 | 48.671 | 2.330 | 19.282 | 1.00 27.02 |
| MOTA | 18852 | CG2 | VAL | 2820 | 49.210 | 4.461 | 20.446 | 1.00 28.43 |
| MOTA | 18853 | С | VAL | 2820 | 45.942 | 2.587 | 19.774 | 1.00 25.78 |
| MOTA | 18854 | 0 | VAL | 2820 | 45.503 | 2.471 | 18.631 | 1.00 27.60 |
| ATOM | 18855 | N | GLU | 2821 | 45.704 | 1.696 | 20.729 | 1.00 24.73 |
| MOTA | 18856 | CA | GLU | 2821 | 44.895 | 0.514 | 20.477 | 1.00 25.30 |
| ATOM | 18857 | CB | GLU | 2821 | 44.782 | -0.321 | 21.755 | 1.00 28.80 |
| ATOM | 18858 | CG | GLU | 2821 | 44.051 | -1.643 | 21.574 | 1.00 32.13 |
| ATOM | 18859 | CD | GLU | 2821 | 43.926 | -2.416 | 22.870 | 1.00 35.13 |
| ATOM | 18860 | | GLU | 2821 | 43.340 | -1.871 | 23.830 | 1.00 36.98 |
| | 18861 | | GLU | 2821 | 44.410 | -3.566 | 22.927 | 1.00 36.11 |
| ATOM | | | | | | | | |
| MOTA | 18862 | С | GLU | 2821 | 43.501 | 0.876 | 19.962 | 1.00 24.62 |
| MOTA | 18863 | 0 | GLU | 2821 | 42.979 | 0.236 | 19.046 | 1.00 21.97 |
| MOTA | 18864 | N | THR | 2822 | 42.900 | 1.905 | 20.549 | 1.00 24.29 |
| ATOM | 18865 | CA | THR | 2822 | 41.568 | 2.336 | 20.141 | 1.00 23.99 |
| ATOM | 18866 | CB | THR | 2822 | 41.021 | 3.415 | 21.099 | 1.00 24.68 |
| ATOM | 18867 | OG1 | THR | 2822 | 40.929 | 2.868 | 22.422 | 1.00 24.15 |
| ATOM | 18868 | CG2 | THR | 2822 | 39.635 | 3.882 | 20.652 | 1.00 23.04 |
| ATOM | 18869 | C | THR | 2822 | 41.590 | 2.876 | 18.715 | 1.00 24.63 |
| ATOM | 18870 | 0 | THR | 2822 | 40.671 | 2.631 | 17.927 | 1.00 21.47 |
| ATOM | 18871 | N | VAL | 2823 | 42.645 | 3.611 | 18.381 | 1.00 23.83 |
| ATOM | 18872 | CA | VAL | 2823 | 42.785 | 4.170 | 17.041 | 1.00 23.79 |
| ATOM | 18873 | CB | VAL | 2823 | 44.002 | 5.116 | 16.961 | 1.00 25.30 |
| | | | | | | | | 1.00 25.93 |
| ATOM | 18874 | CG1 | | 2823 | 44.159 | 5.638 | 15.535 | |
| ATOM | 18875 | CG2 | | 2823 | 43.816 | 6.276 | 17.928 | 1.00 25.50 |
| ATOM | 18876 | С | VAL | 2823 | 42.948 | 3.063 | 16.005 | 1.00 23.15 |
| MOTA | 18877 | 0 | VAL | 2823 | 42.275 | 3.063 | 14.974 | 1.00 21.77 |
| MOTA | 18878 | N | GLN | 2824 | 43.839 | 2.117 | 16.296 | 1.00 24.00 |
| MOTA | 18879 | CA | GLN | 2824 | 44.106 | 1.000 | 15.395 | 1.00 24.92 |
| MOTA | 18880 | CB | GLN | 2824 | 45.156 | 0.068 | 16.005 | 1.00 27.02 |
| ATOM | 18881 | CG | GLN | 2824 | 46.476 | 0.737 | 16.333 | 1.00 33.50 |
| ATOM | 18882 | CD | GLN | 2824 | 47.494 | -0.229 | 16.908 | 1.00 35.79 |
| ATOM | 18883 | OE1 | | 2824 | 47.242 | -0.891 | 17.917 | 1.00 38.12 |
| ATOM | 18884 | NE2 | | 2824 | 48.656 | -0.312 | 16.267 | 1.00 38.24 |
| ATOM | | | | | 42.840 | 0.207 | 15.101 | 1.00 23.85 |
| | 18885 | С | GLN | 2824 | | | | |
| MOTA | 18886 | 0 | GLN | 2824 | 42.518 | -0.057 | 13.946 | 1.00 25.38 |
| MOTA | 18887 | N | MET | 2825 | 42.126 | -0.167 | 16.155 | 1.00 23.02 |
| ATOM | 18888 | CA | MET | 2825 | 40.905 | -0.946 | 16.010 | 1.00 22.80 |
| MOTA | 18889 | CB | MET | 2825 | 40.438 | -1.426 | 17.385 | 1.00 23.09 |
| MOTA | 18890 | CG | MET | 2825 | 41.414 | -2.396 | 18.028 | 1.00 24.85 |
| MOTA | 18891 | SD | MET | 2825 | 40.854 | -3.051 | 19.588 | 1.00 26.27 |
| MOTA | 18892 | CE | MET | 2825 | 39.744 | -4.323 | 19.026 | 1.00 27.47 |
| ATOM | 18893 | С | MET | 2825 | 39.786 | -0.196 | 15.298 | 1.00 20.09 |
| | | | | | | | | |

| ATOM | 18894 | 0 | MET | 2825 | 39.024 | -0.793 | 14.543 | 1.00 19.10 |
|--------------|----------------|----------------|------------|--------------|------------------|------------------|--------|--------------------------|
| ATOM | 18895 | N | LEU | 2826 | 39.685 | 1.109 | 15.537 | 1.00 20.85 |
| ATOM | 18896 | CA | LEU | 2826 | | 1.915 | 14.893 | 1.00 22.61 |
| | 18897 | CB | LEU | 2826 | 38.620 | 3.325 | 15.488 | 1.00 20.71 |
| ATOM | | | | 2826 | 37.867 | 3.457 | 16.819 | 1.00 23.07 |
| ATOM | 18898 | CG | LEU | | | | | 1.00 23.07 |
| ATOM | 18899 | | LEU | 2826 | 38.183 | 4.783 | 17.487 | |
| MOTA | 18900 | | LEU | 2826 | 36.373 | 3.333 | 16.548 | 1.00 21.56 |
| MOTA | 18901 | С | LEU | 2826 | 38.883 | 1.998 | 13.385 | 1.00 24.44 |
| MOTA | 18902 | 0 | LEU | 2826 | 37.944 | 1.870 | 12.597 | 1.00 22.55 |
| MOTA | 18903 | N | THR | 2827 | 40.135 | 2.204 | 12.990 | 1.00 26.28 |
| ATOM | 18904 | CA | THR | 2827 | 40.474 | 2.301 | 11.578 | 1.00 29.53 |
| MOTA | 18905 | CB | THR | 2827 | 41.988 | 2.511 | 11.384 | 1.00 30.21 |
| ATOM | 18906 | OG1 | | 2827 | 42.382 | 3.734 | 12.020 | 1.00 34.27 |
| ATOM | 18907 | | THR | 2827 | 42.327 | 2.588 | 9.901 | 1.00 33.86 |
| ATOM | 18908 | C | THR | 2827 | 40.034 | 1.060 | 10.795 | 1.00 27.89 |
| | 18909 | 0 | THR | 2827 | 39.349 | 1.173 | 9.779 | 1.00 28.82 |
| ATOM | | | | | | | 11.268 | 1.00 28.30 |
| ATOM | 18910 | N | GLU | 2828 | 40.416 | -0.121 | | |
| ATOM | 18911 | CA | GLU | 2828 | 40.041 | -1.350 | 10.580 | 1.00 28.55 |
| MOTA | 18912 | CB | GLU | 2828 | 40.775 | -2.548 | 11.179 | 1.00 30.32 |
| MOTA | 18913 | CG | GLU | 2828 | 41.107 | -2.404 | 12.638 | 1.00 31.98 |
| MOTA | 18914 | CD | GLU | 2828 | 41.836 | -3.614 | 13.180 | 1.00 32.11 |
| ATOM | 18915 | OE1 | GLU | 2828 | 42.836 | -4.041 | 12.564 | 1.00 32.16 |
| ATOM | 18916 | OE2 | GLU | 2828 | 41.415 | -4.134 | 14.235 | 1.00 30.79 |
| ATOM | 18917 | С | GLU | 2828 | 38.540 | -1.588 | 10.592 | 1.00 27.06 |
| ATOM | 18918 | 0 | GLU | 2828 | 38.030 | -2.412 | 9.831 | 1.00 27.55 |
| ATOM | 18919 | N | ARG | 2829 | 37.829 | -0.857 | 11.444 | 1.00 23.40 |
| ATOM | 18920 | CA | ARG | 2829 | 36.384 | -0.997 | 11.513 | 1.00 22.00 |
| | | | | | | | 12.973 | 1.00 20.32 |
| MOTA | 18921 | CB | ARG | 2829 | 35.931 | -1.037 | | |
| ATOM | 18922 | CG | ARG | 2829 | 36.241 | -2.378 | 13.629 | 1.00 19.39 |
| MOTA | 18923 | CD | ARG | 2829 | 36.285 | -2.294 | 15.140 | 1.00 18.70 |
| MOTA | 18924 | NE | ARG | 2829 | 36.650 | -3.585 | 15.719 | 1.00 16.89 |
| ATOM | 18925 | CZ | ARG | 2829 | 37.869 | -4.112 | 15.666 | 1.00 17.72 |
| MOTA | 18926 | NH1 | ARG | 2829 | 38.856 | -3.459 | 15.065 | 1.00 16.97 |
| MOTA | 18927 | NH2 | ARG | 2829 | 38.102 | -5.303 | 16.201 | 1.00 21.33 |
| ATOM | 18928 | С | ARG | 2829 | 35.674 | 0.104 | 10.739 | 1.00 20.80 |
| ATOM | 18929 | Ó | ARG | 2829 | 34.536 | 0.458 | 11.040 | 1.00 19.63 |
| ATOM | 18930 | N | ALA | 2830 | 36.368 | 0.642 | 9.737 | 1.00 21.90 |
| ATOM | 18931 | CA | ALA | 2830 | 35.825 | 1.680 | 8.856 | 1.00 21.97 |
| | 18932 | CB | ALA | 2830 | 34.474 | 1.223 | 8.305 | 1.00 22.04 |
| ATOM | | | | | 35.690 | | 9.435 | 1.00 22.69 |
| MOTA | 18933 | C | ALA | 2830 | | 3.086 | | |
| MOTA | 18934 | 0 | ALA | 2830 | 35.042 | 3.937 | 8.828 | 1.00 22.61 |
| MOTA | 18935 | N | VAL | 2831 | 36.297 | 3.341 | 10.589 | 1.00 22.14 |
| MOTA | 18936 | CA | VAL | 2831 | 36.194 | 4.662 | 11.194 | 1.00 22.55 |
| ATOM | 18937 | CB | VAL | 2831 | 35.679 | 4.570 | 12.651 | 1.00 23.25 |
| MOTA | 18938 | CG1 | VAL | 2831 | 35.612 | 5.957 | 13.264 | 1.00 22.11 |
| MOTA | 18939 | CG2 | VAL | 2831 | 34.300 | 3.910 | 12.684 | 1.00 21.29 |
| MOTA | 18940 | С | VAL | 2831 | 37.520 | 5.427 | 11.207 | 1.00 22.41 |
| MOTA | 18941 | 0 | VAL | 2831 | 38.439 | 5.071 | 11.940 | 1.00 21.58 |
| MOTA | 18942 | N | PRO | 2832 | 37.634 | 6.490 | 10.389 | 1.00 22.74 |
| ATOM | 18943 | CD | PRO | 2832 | 36.681 | 6.962 | 9.370 | 1.00 23.21 |
| ATOM | 18944 | CA | PRO | 2832 | 38.870 | 7.279 | 10.350 | 1.00 23.36 |
| ATOM | 18945 | CB - | | 2832 | 38.710 | 8.110 | 9.081 | 1.00 24.93 |
| | | | | | | | 9.011 | 1.00 24.33 |
| ATOM | 18946 | CG | PRO | 2832 | 37.244 | 8.323 | | |
| ATOM | 18947 | C | PRO | 2832 | 38.961 | 8.129 | 11.611 | 1.00 23.38 |
| MOTA | 18948 | 0 | PRO | 2832 | 37.954 | 8.644 | 12.093 | 1.00 20.50 |
| MOTA | 18949 | N | VAL | 2833 | 40.169 | 8.274 | 12.143 | 1.00 23.46 |
| ATOM | 18950 | CA | VAL | 2833 | 40.352 | 9.035 | 13.368 | 1.00 24.56 |
| ATOM | 18951 | CB | VAL | 2833 | 40.985 | 8.147 | 14.466 | 1.00 25.29 |
| MOTA | 18952 | CG1 | VAL | 2833 | 41.061 | 8.909 | 15.778 | 1.00 26.10 |
| ATOM | 18953 | CG2 | VAL | 2833 | 40.167 | 6.869 | 14.638 | 1.00 26.15 |
| ATOM | 18954 | С | VAL | 2833 | 41.206 | 10.284 | 13.203 | 1.00 26.06 |
| MOTA | 18955 | 0 | VAL | 2833 | 42.156 | 10.307 | 12.420 | 1.00 22.96 |
| ATOM | 18956 | N | CYS | 2834 | 40.842 | 11.325 | 13.943 | 1.00 26.64 |
| MOTA | 18957 | CA | CYS | 2834 | 41.580 | 12.583 | 13.943 | 1.00 27.09 |
| ATOM | 18958 | CB | CYS | 2834 | 40.683 | 13.755 | 13.553 | 1.00 27.30 |
| | | | | | | | 13.665 | 1.00 27.30 |
| ATOM | 18959 | SG | CYS | 2834 | 41.516 | 15.369 | | |
| MOTA | 18960 | C | CYS | 2834 | 42.098 | 12.794 | 15.358 | 1.00 28.85 |
| MOTA | 18961 | 0 | CYS | 2834 | 41.316 | 12.957 | 16.297 | 1.00 28.83 |
| MOTA | 18962 | N | GLY | 2835 | 43.418 | 12.776 | 15.508 | 1.00 29.22 |
| MOTA | 18963 | CA | GLY | 2835 | 44.014 | 12.970 | 16.816 | 1.00 29.92 |
| MOTA | 18964 | С | GLY | 2835 | 43.832 | 14.382 | 17.336 | 1.00 30.47 |
| MOTA | 18965 | 0 | GLY | 2835 | 43.460 | 15.288 | 16.590 | 1.00 28.61 |
| MOTA | | | HIS | 2836 | 44.100 | 14.561 | 18.624 | 1.00 31.84 |
| AION | 18966 | N | 1113 | | | | | |
| | | | | | 43.971 | | 19.274 | 1.00 35.35 |
| MOTA | 18967 | CA | HIŞ | 2836 | 43.971 | 15.860 | | 1.00 35.35 |
| MOTA MOTA | 18967 18968 | CA CB | HIS HIS | 2836 2836 | 43.971 42.553 | 15.860 16.033 | 19.816 | 1.00 35.35 1.00 36.73 |
| MOTA | 18967 | CA CB CG | HIŞ | 2836 | 43.971 | 15.860 | | 1.00 35.35 |

| MOTA | 18971 | ND1 | HIS | 2836 | 41.313 | 18.226 | 19.837 | 1.00 39.91 |
|------|-------|--------|------------|-------|--------|--------|--------|------------|
| ATOM | 18972 | CE1 | HIS | 2836 | 41.274 | 19.350 | 20.531 | 1.00 41.13 |
| ATOM | 18973 | | HIS | 2836 | 42.180 | 19.278 | 21.490 | 1.00 41.39 |
| | | | HIS | 2836 | 44.973 | 15.941 | 20.420 | 1.00 36.62 |
| ATOM | 18974 | С | | | | | | |
| ATOM | 18975 | 0 | HIS | 2836 | 44.800 | 15.291 | 21.452 | 1.00 34.99 |
| MOTA | 18976 | N | LEU | 2837 | 46.018 | 16.742 | 20.231 | 1.00 38.21 |
| ATOM | 18977 | CA | LEU | 2837 | 47.059 | 16.905 | 21.239 | 1.00 41.31 |
| ATOM | 18978 | CB | LEU | 2837 | 48.365 | 16.279 | 20.745 | 1.00 40.92 |
| ATOM | 18979 | CG | LEU | 2837 | 48.343 | 14.765 | 20.510 | 1.00 40.97 |
| ATOM | 18980 | CD1 | LEU | 2837 | 49.609 | 14.330 | 19.794 | 1.00 41.01 |
| | | CD2 | LEU | 2837 | 48.201 | 14.051 | 21.840 | 1.00 41.35 |
| ATOM | 18981 | | | | | | | 1.00 41.33 |
| MOTA | 18982 | C | LEU | 2837 | 47.285 | 18.377 | 21.557 | |
| MOTA | 18983 | 0 | LEU | 2837 | 46.981 | 19.249 | 20.745 | 1.00 43.31 |
| ATOM | 18984 | N | GLY | 2838 | 47.820 | 18.647 | 22.743 | 1.00 46.60 |
| MOTA | 18985 | CA | GLY | 2838. | 48.077 | 20.018 | 23.141 | 1.00 50.65 |
| ATOM | 18986 | С | GLY | 2838 | 47.359 | 20.378 | 24.425 | 1.00 53.60 |
| ATOM | 18987 | 0 | GLY | 2838 | 47.800 | 20.013 | 25.514 | 1.00 54.57 |
| ATOM | 18988 | N | LEU | 2839 | 46.246 | 21.092 | 24.297 | 1.00 56.02 |
| | 18989 | CA | LEU | 2839 | 45.466 | 21.503 | 25.457 | 1.00 58.56 |
| ATOM | | | | | | | | 1.00 58.83 |
| MOTA | 18990 | CB | LEU | 2839 | 45.363 | 23.032 | 25.490 | |
| MOTA | 18991 | CG | LEU | 2839 | 45.049 | 23.710 | 26.827 | 1.00 59.71 |
| MOTA | 18992 | CD1 | LEU | 2839 | 45.256 | 25.209 | 26.685 | 1.00 60.17 |
| MOTA | 18993 | CD2 | LEU | 2839 | 43.631 | 23.394 | 27.263 | 1.00 59.46 |
| MOTA | 18994 | С | LEU | 2839 | 44.074 | 20.875 | 25.377 | 1.00 60.00 |
| ATOM | 18995 | 0 | LEU | 2839 | 43.142 | 21.473 | 24.843 | 1.00 60.93 |
| ATOM | 18996 | N | THR | 2840 | 43.944 | 19.663 | 25.910 | 1.00 61.24 |
| ATOM | 18997 | CA | THR | 2840 | 42.672 | 18.946 | 25.892 | 1.00 62.45 |
| | | | THR | 2840 | 42.879 | 17.438 | 26.157 | 1.00 62.30 |
| MOTA | 18998 | CB | | | | | | |
| MOTA | 18999 | OG1 | THR | 2840 | 43.477 | 17.254 | 27.446 | 1.00 62.47 |
| ATOM | 19000 | CG2 | THR | 2840 | 43.782 | 16.831 | 25.094 | 1.00 62.36 |
| ATOM | 19001 | С | THR | 2840 | 41.688 | 19.493 | 26.925 | 1.00 63.01 |
| MOTA | 19002 | 0 | THR | 2840 | 41.915 | 19.383 | 28.131 | 1.00 63.56 |
| MOTA | 19003 | N | PRO | 2841 | 40.577 | 20.090 | 26.460 | 1.00 63.41 |
| ATOM | 19004 | CD | PRO | 2841 | 40.230 | 20.321 | 25.046 | 1.00 63.65 |
| ATOM | 19005 | CA | PRO | 2841 | 39.553 | 20.658 | 27.343 | 1.00 63.37 |
| | | CB | PRO | 2841 | 38.678 | 21.457 | 26.380 | 1.00 63.72 |
| MOTA | 19006 | | | | | | | |
| MOTA | 19007 | CG | PRO | 2841 | 38.754 | 20.648 | 25.127 | 1.00 64.24 |
| MOTA | 19008 | С | PRO | 2841 | 38.756 | 19.614 | 28.127 | 1.00 62.86 |
| MOTA | 19009 | 0 | PRO | 2841 | 38.222 | 19.911 | 29.196 | 1.00 62.53 |
| MOTA | 19010 | N | GLN | 2842 | 38.676 | 18.397 | 27.594 | 1.00 62.50 |
| MOTA | 19011 | CA | GLN | 2842 | 37.945 | 17.320 | 28.258 | 1.00 62.12 |
| MOTA | 19012 | CB | GLN | 2842 | 37.873 | 16.081 | 27.359 | 1.00 62.10 |
| ATOM | 19013 | CG | GLN | 2842 | 36.798 | 16.147 | 26.282 | 1.00 61.81 |
| MOTA | 19014 | CD | GLN | 2842 | 36.712 | 14.871 | 25.465 | 1.00 61.57 |
| | 19015 | | GLN | 2842 | 36.650 | 13.772 | 26.016 | 1.00 61.29 |
| MOTA | | | | | | | | |
| MOTA | 19016 | NE2 | GLN | 2842 | 36.698 | 15.012 | 24.145 | 1.00 61.54 |
| MOTA | 19017 | C . | GLN | 2842 | 38.583 | 16.942 | 29.591 | 1.00 61.81 |
| ATOM | 19018 | 0 | GLN | 2842 | 37.955 | 16.293 | 30.429 | 1.00 61.09 |
| MOTA | 19019 | N | SER | 2843 | 39.833 | 17.352 | 29.781 | 1.00 61.46 |
| MOTA | 19020 | CA | SER | 2843 | 40.557 | 17.060 | 31.012 | 1.00 61.52 |
| MOTA | 19021 | CB | SER | 2843 | 41.890 | 16.381 | 30.689 | 1.00 61.26 |
| MOTA | 19022 | OG | SER | 2843 | | 15.191 | 29.947 | 1.00 61.14 |
| ATOM | 19023 | C | SER | 2843 | 40.810 | 18.342 | 31.798 | 1.00 61.57 |
| | 19024 | | | 2843 | 41.905 | 18.555 | 32:320 | 1.00 62.21 |
| ATOM | | O N | SER VAL | 2844 | 39.790 | 19.191 | 31.879 | 1.00 61.40 |
| ATOM | 19025 | | | | | | | |
| ATOM | 19026 | CA | VAL | 2844 | 39.894 | 20.460 | 32.593 | 1.00 61.08 |
| MOTA | 19027 | CB | VAL | 2844 | 38.645 | 21.343 | 32.336 | 1.00 60.81 |
| MOTA | 19028 | CG1 | VAL | 2844 | 37.385 | 20.609 | 32.764 | 1.00 60.34 |
| ATOM | 19029 | CG2 | VAL | 2844 | 38.775 | 22.662 | 33.080 | 1.00 60.79 |
| MOTA | 19030 | С | VAL | 2844 | 40.066 | 20.259 | 34.101 | 1.00 61.01 |
| ATOM | 19031 | 0 | VAL | 2844 | 40.803 | 21.001 | 34.754 | 1.00 60.58 |
| ATOM | 19032 | N | ASN | 2845 | 39.389 | 19.251 | 34.644 | 1.00 61.15 |
| ATOM | 19033 | CA | ASN | 2845 | 39.460 | 18.947 | 36.071 | 1.00 61.73 |
| ATOM | 19033 | CB | ASN | 2845 | 38.364 | 17.946 | 36.449 | 1.00 60.56 |
| | | | ASN | | 36.970 | 18.499 | 36.230 | 1.00 59.61 |
| MOTA | 19035 | CG | | 2845 | | | | 1.00 59.61 |
| ATOM | 19036 | | ASN | 2845 | 36.548 | 19.436 | 36.907 | |
| MOTA | 19037 | ND2 | ASN | 2845 | 36.249 | 17.924 | 35.275 | 1.00 59.70 |
| MOTA | 19038 | С | ASN | 2845 | 40.821 | 18.388 | 36.475 | 1.00 62.60 |
| MOTA | 19039 | 0 | ASN | 2845 | 41.296 | 18.629 | 37.586 | 1.00 62.03 |
| MOTA | 19040 | N | ILE | 2846 | 41.441 | 17.636 | 35.570 | 1.00 64.05 |
| MOTA | 19041 | CA | ILE | 2846 | 42.750 | 17.046 | 35.831 | 1.00 65.55 |
| ATOM | 19042 | CB | ILE | 2846 | 43.208 | 16.151 | 34.651 | 1.00 65.57 |
| MOTA | 19043 | CG2 | ILE | 2846 | 44.609 | 15.612 | 34.915 | 1.00 65.70 |
| ATOM | 19043 | CG1 | ILE | 2846 | 42.223 | 14.995 | 34.453 | 1.00 65.59 |
| | | | | | | | | 1.00 65.39 |
| ATOM | 19045 | CD1 | ILE | 2846 | 42.118 | 14.057 | 35.643 | |
| ATOM | 19046 | C | ILE | 2846 | 43.795 | 18.137 | 36.051 | 1.00 66.57 |
| ATOM | 19047 | О | ILE | 2846 | 44.490 | 18.150 | 37.066 | 1.00 66.67 |
| | | | | | | | | |

| ATOM | 19048 | N | PHE | 2847 | 43.896 | 19.053 | 35.092 | 1.00 67.71 |
|--------------|-------|------|------|------|--------|--------|--------|------------|
| MOTA | 19049 | CA | PHE | 2847 | 44.855 | 20.149 | 35.172 | 1.00 68.89 |
| ATOM | 19050 | CB | PHE | 2847 | 45.158 | 20.684 | 33.771 | 1.00 69.22 |
| MOTA | 19051 | CG | PHE | 2847 | 45.618 | 19.630 | 32.807 | 1.00 69.88 |
| ATOM | 19052 | CD1 | PHE | 2847 | 46.776 | 18.899 | 33.055 | 1.00 70.09 |
| ATOM | 19053 | CD2 | PHE | 2847 | 44.892 | 19.365 | 31.649 | 1.00 70.08 |
| ATOM | 19054 | CE1 | PHE | 2847 | 47.206 | 17.918 | 32.164 | 1.00 70.40 |
| MOTA | 19055 | CE2 | PHE | 2847 | 45.311 | 18.387 | 30.751 | 1.00 70.36 |
| MOTA | 19056 | CZ | PHE | 2847 | 46.471 | 17.661 | 31.009 | 1.00 70.74 |
| MOTA | 19057 | С | PHE | 2847 | 44.333 | 21.284 | 36.050 | 1.00 69.49 |
| ATOM | 19058 | 0 | PHE | 2847 | 45.040 | 22.262 | 36.299 | 1.00 69.68 |
| MOTA | 19059 | N | GLY | 2848 | 43.094 | 21.149 | 36.513 | 1.00 69.83 |
| MOTA | 19060 | CA | GLY | 2848 | 42.502 | 22.174 | 37.353 | 1.00 70.24 |
| MOTA | 19061 | С | GLY | 2848 | 42.298 | 23.478 | 36.605 | 1.00 70.50 |
| MOTA | 19062 | 0 | GLY | 2848 | 42.086 | 24.528 | 37.212 | 1.00 70.31 |
| ATOM | 19063 | N | GLY | 2849 | 42.363 | 23.407 | 35.280 | 1.00 71.04 |
| ATOM | 19064 | CA | GLY | 2849 | 42.185 | 24.591 | 34.459 | 1.00 71.60 |
| MOTA | 19065 | С | GLY | 2849 | 42.700 | 24.367 | 33.051 | 1.00 72.16 |
| MOTA | 19066 | 0 | GLY | 2849 | 42.776 | 23.228 | 32.589 | 1.00 72.14 |
| ATOM | 19067 | N | TYR | 2850 | 43.056 | 25.450 | 32.366 | 1.00 72.95 |
| ATOM | 19068 | CA | TYR | 2850 | 43.570 | 25.353 | 31.005 | 1.00 73.65 |
| ATOM | 19069 | CB | TYR | 2850 | 42.679 | 26.142 | 30.038 | 1.00 73.69 |
| ATOM | 19070 | CG | TYR | 2850 | 41.257 | 25.633 | 29.969 | 1.00 74.01 |
| ATOM | 19071 | CD1 | TYR | 2850 | 40.353 | 25.887 | 31.001 | 1.00 74.35 |
| ATOM | 19072 | CE1 | TYR | 2850 | 39.050 | 25.395 | 30.956 | 1.00 74.49 |
| ATOM | 19073 | CD2 | | 2850 | 40.821 | 24.871 | 28.883 | 1.00 74.02 |
| ATOM | 19074 | CE2 | TYR | 2850 | 39.520 | 24.373 | 28.828 | 1.00 74.41 |
| | 19075 | CZ | TYR | 2850 | 38.641 | 24.639 | 29.868 | 1.00 74.41 |
| MOTA | | OH | TYR | 2850 | 37.355 | 24.039 | 29.826 | 1.00 74.00 |
| ATOM ATOM | 19076 | | | 2850 | 45.007 | 25.853 | 30.907 | 1.00 73.22 |
| | 19077 | C | TYR | | | | 30.847 | 1.00 74.16 |
| MOTA | 19078 | 0 | TYR | 2850 | 45.256 | 27.059 | | |
| MOTA | 19079 | N | LYS | 2851 | 45.947 | 24.913 | 30.892 | |
| ATOM | 19080 | CA | LYS | 2851 | 47.369 | 25.229 | 30.801 | |
| MOTA | 19081 | CB | LYS | 2851 | 48.166 | 24.299 | 31.719 | 1.00 75.40 |
| MOTA | 19082 | CG | LYS | 2851 | 47.704 | 24.325 | 33.168 | 1.00 75.61 |
| MOTA | 19083 | CD | LYS | 2851 | 48.399 | 23.258 | 33.998 | 1.00 75.38 |
| MOTA | 19084 | CE | LYS | 2851 | 47.875 | 23.249 | 35.426 | 1.00 75.26 |
| MOTA | 19085 | NZ | LYS | 2851 | 48.476 | 22.152 | 36.233 | 1.00 74.92 |
| MOTA | 19086 | С | LYS | 2851 | 47.845 | 25.070 | 29.358 | 1.00 75.66 |
| MOTA | 19087 | 0 | LYS | 2851 | 47.572 | 24.057 | 28.714 | 1.00 76.01 |
| MOTA | 19088 | N | VAL | 2852 | 48.557 | 26.073 | 28.857 | 1.00 75.85 |
| MOTA | 19089 | CA | VAL | 2852 | 49.062 | 26.043 | 27.489 | 1.00 76.08 |
| MOTA | 19090 | CB | VAL | 2852 | 49.525 | 27.448 | 27.036 | 1.00 75.99 |
| MOTA | 19091 | | | 2852 | 49.922 | 27.421 | 25.568 | 1.00 75.65 |
| MOTA | 19092 | CG2 | VAL | 2852 | 48.417 | 28.463 | 27.273 | 1.00 75.82 |
| MOTA | 19093 | C | VAL | 2852 | 50.234 | 25.074 | 27.346 | 1.00 76.39 |
| MOTA | 19094 | 0 | VAL | 2852 | 51.395 | 25.484 | 27.394 | 1.00 76.33 |
| MOTA | 19095 | N | GLN | 2853 | 49.930 | 23.789 | 27.173 | 1.00 76.70 |
| MOTA | 19096 | CA | GLN | 2853 | 50.971 | 22.777 | 27.016 | 1.00 77.12 |
| MOTA | 19097 | CB | GLN | 2853 | 50.360 | 21.375 | 26.913 | 1.00 77.23 |
| MOTA | 19098 | CG | GLN | 2853 | 50.094 | 20.680 | 28.247 | 1.00 76.94 |
| MOTA | 19099 | CD | GLN | 2853 | 48.944 | 21.289 | 29.021 | 1.00 76.79 |
| MOTA | 19100 | OE1 | GLN | 2853 | 47.825 | 21.379 | 28.519 | 1.00 76.67 |
| MOTA | 19101 | NE2 | GLN | 2853 | 49.210 | 21.699 | 30.256 | 1.00 77.11 |
| MOTA | 19102 | С | GLN | 2853 | 51.813 | 23.054 | 25.774 | 1.00 77.33 |
| MOTA | 19103 | 0 | GLN | 2853 | 51.369 | 23.740 | 24.853 | 1.00 77.15 |
| MOTA | 19104 | N | GLY | 2854 | 53.027 | 22.514 | 25.755 | 1.00 77.75 |
| ATOM | 19105 | CA | GLY | 2854 | 53.911 | 22.717 | 24.622 | 1.00 78.29 |
| MOTA | 19106 | C | GLY | 2854 | 55.254 | 23.293 | 25.028 | 1.00 78.76 |
| MOTA | 19107 | 0 | GLY | 2854 | 56.190 | 23.331 | 24.228 | 1.00 78.78 |
| MOTA | 19108 | N | ARG | 2855 | 55.348 | 23.744 | 26.276 | 1.00 79.02 |
| MOTA | 19109 | CA | ARG | 2855 | 56.584 | 24.320 | 26.800 | 1.00 79.07 |
| ATOM | 19110 | CB | ARG | 2855 | 56.271 | 25.282 | 27.954 | 1.00 79.32 |
| MOTA | 19111 | CG | ARG | 2855 | 55.397 | 26.471 | 27.572 | 1.00 79.76 |
| MOTA | 19112 | CD | ARG | 2855 | 56.115 | 27.420 | 26.620 | 1.00 80.09 |
| MOTA | 19113 | NE | ARG | 2855 | 55.254 | 28.516 | 26.174 | 1.00 80.24 |
| ATOM | 19114 | | ARG | 2855 | 54.727 | 29.437 | 26.976 | 1.00 79.98 |
| ATOM | 19115 | NH1 | | 2855 | 54.968 | 29.406 | 28.280 | 1.00 79.86 |
| ATOM | 19116 | NH2 | | 2855 | 53.956 | 30.393 | 26.473 | 1.00 79.79 |
| ATOM | 19117 | C | ARG | 2855 | 57.524 | 23.222 | 27.293 | 1.00 78.89 |
| ATOM | 19118 | o | ARG | 2855 | 57.079 | 22.176 | 27.767 | 1.00 78.88 |
| ATOM | 19119 | N | GLY | 2856 | 58.826 | 23.468 | 27.179 | 1.00 78.53 |
| ATOM | 19120 | CA | GLY | 2856 | 59.805 | 22.492 | 27.619 | 1.00 78.02 |
| MOTA | 19121 | C | GLY | 2856 | 60.118 | 21.456 | 26.557 | 1.00 77.79 |
| MOTA | 19122 | 0 | GLY | 2856 | 59.439 | 21.382 | 25.532 | 1.00 77.80 |
| ATOM | 19123 | N | ASP | 2857 | 61.150 | 20.655 | 26.802 | 1.00 77.36 |
| MOTA | 19124 | CA | ASP | 2857 | 61.555 | 19.616 | 25.861 | 1.00 76.70 |
| | | U- 1 | -101 | | -2.555 | | | |

| ATOM | 19125 | CB | ASP | 2857 | 63.077 | 19.446 | 25.875 | 1.00 76.96 |
|------|-------|-----------|-----|------|------------------|------------------|------------------|--------------------------|
| ATOM | 19126 | CG | ASP | 2857 | 63.801 | 20.634 | 25.273 | 1.00 77.36 |
| | | | ASP | 2857 | 63.527 | 20.962 | 24.099 | 1.00 77.51 |
| MOTA | 19127 | | | | | | | 1.00 77.38 |
| MOTA | 19128 | | ASP | 2857 | 64.644 | 21.235 | 25.971 | |
| MOTA | 19129 | С | ASP | 2857 | 60.892 | 18.282 | 26.177 | 1.00 75.97 |
| MOTA | 19130 | 0 | ASP | 2857 | 60.391 | 17.606 | 25.280 | 1.00 76.56 |
| MOTA | 19131 | N | GLU | 2858 | 60.896 | 17.901 | 27.450 | 1.00 74.75 |
| ATOM | 19132 | CA | GLU | 2858 | 60.288 | 16.644 | 27.863 | 1.00 73.64 |
| ATOM | 19133 | CB | GLU | 2858 | 60.368 | 16.484 | 29.383 | 1.00 74.08 |
| ATOM | 19134 | CG | GLU | 2858 | 59.765 | 15.184 | 29.899 | 1.00 74.86 |
| | | | | | | | 31.408 | 1.00 75.46 |
| MOTA | 19135 | CD | GLU | 2858 | 59.856 | 15.050 | | |
| MOTA | 19136 | OE1 | | 2858 | 60.986 | 15.074 | 31.941 | 1.00 75.97 |
| MOTA | 19137 | OE2 | GLU | 2858 | 58.798 | 14.918 | 32.061 | 1.00 75.55 |
| MOTA | 19138 | С | GLU | 2858 | 58.831 | 16.596 | 27.416 | 1.00 72.68 |
| ATOM | 19139 | 0 | GLU | 2858 | 58.319 | 15.537 | 27.056 | 1.00 72.94 |
| ATOM | 19140 | N | ALA | 2859 | 58.172 | 17.751 | 27.441 | 1.00 71.17 |
| MOTA | 19141 | CA | ALA | 2859 | 56.774 | 17.848 | 27.036 | 1.00 69.66 |
| ATOM | 19142 | СВ | ALA | 2859 | 56.091 | 18.987 | 27.786 | 1.00 69.37 |
| | | | | | | | 25.534 | 1.00 68.42 |
| MOTA | 19143 | C | ALA | 2859 | 56.682 | 18.083 | | |
| MOTA | 19144 | 0 | ALA | 2859 | 55.790 | 17.560 | 24.864 | 1.00 68.24 |
| MOTA | 19145 | N | GLY | 2860 | 57.613 | 18.876 | 25.014 | 1.00 67.04 |
| MOTA | 19146 | CA | GLY | 2860 | 57.628 | 19.171 | 23.595 | 1.00 65.45 |
| MOTA | 19147 | С | GLY | 2860 | 57.836 | 17.929 | 22.753 | 1.00 64.41 |
| MOTA | 19148 | 0 | GLY | 2860 | 57.153 | 17.734 | 21.748 | 1.00 64.15 |
| ATOM | 19149 | N | ASP | 2861 | 58.782 | 17.087 | 23.160 | 1.00 63.48 |
| | 19150 | CA | ASP | 2861 | 59.070 | 15.856 | 22.433 | 1.00 62.53 |
| MOTA | | | | | 60.439 | 15.302 | 22.831 | 1.00 62.67 |
| MOTA | 19151 | CB | ASP | 2861 | | | | |
| ATOM | 19152 | CG | ASP | 2861 | 61.562 | 16.288 | 22.579 | 1.00 63.21 |
| MOTA | 19153 | | ASP | 2861 | 61.615 | 16.865 | 21.471 | 1.00 62.95 |
| MOTA | 19154 | OD2 | ASP | 2861 | 62.397 | 16.478 | 23.487 | 1.00 63.46 |
| MOTA | 19155 | С | ASP | 2861 | 57.999 | 14.811 | 22.716 | 1.00 61.69 |
| ATOM | 19156 | 0 | ASP | 2861 | 57.830 | 13.860 | 21.953 | 1.00 61.58 |
| ATOM | 19157 | N | GLN | 2862 | 57.285 | 14.992 | 23.822 | 1.00 60.47 |
| ATOM | 19158 | CA | GLN | 2862 | 56.221 | 14.073 | 24.207 | 1.00 59.44 |
| | | | | | 55.729 | 14.389 | 25.620 | 1.00 59.54 |
| MOTA | 19159 | CB | GLN | 2862 | | | | |
| ATOM | 19160 | CG | GLN | 2862 | 54.527 | 13.569 | 26.050 | 1.00 59.67 |
| MOTA | 19161 | CD | GLN | 2862 | 54.800 | 12.080 | 26.016 | 1.00 59.97 |
| MOTA | 19162 | OE1 | GLN | 2862 | 55.653 | 11.578 | 26.748 | 1.00 60.86 |
| MOTA | 19163 | NE2 | GLN | 2862 | 54.078 | 11.366 | 25.160 | 1.00 59.63 |
| MOTA | 19164 | С | GLN | 2862 | 55.061 | 14.194 | 23.227 | 1.00 58.25 |
| ATOM | 19165 | 0 | GLN | 2862 | 54.494 | 13.193 | 22.797 | 1.00 58.14 |
| ATOM | 19166 | N | LEU | 2863 | 54.712 | 15.429 | 22.884 | 1.00 57.06 |
| ATOM | 19167 | CA | LEU | 2863 | 53.625 | 15.679 | 21.951 | 1.00 56.74 |
| | | | | 2863 | 53.350 | 17.181 | 21.844 | 1.00 57.27 |
| ATOM | 19168 | CB | LEU | | | | | |
| MOTA | 19169 | CG | LEU | 2863 | 52.854 | 17.884 | 23.111 | 1.00 57.78 |
| ATOM | 19170 | CD1 | | 2863 | 52.796 | 19.385 | 22.873 | 1.00 58.08 |
| ATOM | 19171 | CD2 | LEU | 2863 | 51.485 | 17.347 | 23.497 | 1.00 57.79 |
| MOTA | 19172 | C | LEU | 2863 | 53.988 | 15.128 | 20.580 | 1.00 56.01 |
| ATOM | 19173 | 0 | LEU | 2863 | 53.163 | 14.504 | 19.911 | 1.00 56.51 |
| ATOM | 19174 | N | LEU | 2864 | 55.230 | 15.358 | 20.168 | 1.00 54.58 |
| ATOM | 19175 | CA | LEU | 2864 | 55.700 | 14.882 | 18.873 | 1.00 53.21 |
| ATOM | 19176 | CB | LEH | | | 15.427 | | 1.00 53.69 |
| | | | | 2001 | | 15.447 | 17.145 | 1.00 54.10 |
| ATOM | 19177 | CG CD1 | LEU | 2864 | 57.598 58.822 | 16.342 | 17.143 | 1.00 54.10 |
| MOTA | 19178 | | LEU | 2864 | | | | |
| MOTA | 19179 | | LEU | 2864 | 57.911 | 14.043 | 16.669 | 1.00 53.90 |
| MOTA | 19180 | C | LEU | 2864 | 55.707 | 13.355 | 18.879 | 1.00 51.65 |
| MOTA | 19181 | 0 | LEU | 2864 | 55.486 | 12.717 | 17.847 | 1.00 50.82 |
| MOTA | 19182 | N | SER | 2865 | 55.954 | 12.781 | 20.053 | 1.00 49.04 |
| MOTA | 19183 | CA | SER | 2865 | 55.975 | 11.332 | 20.209 | 1.00 47.06 |
| ATOM | 19184 | CB | SER | 2865 | 56.542 | 10.954 | 21.581 | 1.00 46.62 |
| ATOM | 19185 | OG | SER | 2865 | 56.593 | 9.548 | 21.749 | 1.00 44.01 |
| ATOM | 19186 | C | SER | 2865 | 54.561 | 10.774 | 20.062 | 1.00 45.80 |
| ATOM | 19187 | 0 | SER | 2865 | 54.346 | 9.778 | 19.367 | 1.00 44.53 |
| | | | | | | | | |
| ATOM | 19188 | N | ASP | | 53.600 | 11.417 | 20.720 | 1.00 44.91 |
| ATOM | 19189 | CA | ASP | 2866 | 52.210 | 10.976 | 20.645 | 1.00 44.58 |
| MOTA | 19190 | CB | ASP | 2866 | 51.329 | 11.752 | 21.631 | 1.00 45.13 |
| MOTA | 19191 | CG | ASP | 2866 | 51.719 | 11.514 | 23.080 | 1.00 45.03 |
| MOTA | 19192 | OD1 | ASP | 2866 | 51.989 | 10.352 | 23.452 | 1.00 44.80 |
| ATOM | 19193 | | ASP | 2866 | 51.740 | 12.489 | 23.855 | 1.00 46.12 |
| ATOM | 19194 | C | ASP | 2866 | 51.687 | 11.180 | 19.229 | 1.00 44.24 |
| ATOM | 19195 | Ö | ASP | 2866 | 50.975 | 10.329 | 18.694 | 1.00 45.01 |
| ATOM | 19196 | . N | ALA | 2867 | 52.043 | 12.310 | 18.626 | 1.00 42.65 |
| | | | | | | | | |
| MOTA | 19197 | CA | ALA | 2867 | 51.612 | 12.610 | 17.267 | 1.00 41.30 |
| | | | ALA | 2867 | 52.178 | 13.952 | 16.820 | 1.00 40.89 |
| MOTA | 19198 | CB | | | | | | |
| MOTA | 19199 | С | ALA | 2867 | 52.077 | 11.498 | 16.328 | 1.00 40.67 |
| | | | | | 52.077 51.325 | 11.498 11.051 | 16.328 15.461 | 1.00 40.67 1.00 38.64 |
| MOTA | 19199 | С | ALA | 2867 | 52.077 | 11.498 | 16.328 | 1.00 40.67 |

| ATOM | 19202 | CA | LEU | 2868 | 53.862 | 9.982 | 15.674 | 1.00 39.13 |
|--------------|----------------|----------------|------------|--------------|------------------|----------------|------------------|--------------------------|
| ATOM | 19203 | СВ | LEU | 2868 | 55.375 | 9.852 | 15.881 | 1.00 39.80 |
| ATOM | 19204 | CG | LEU | 2868 | 56.263 | 10.908 | 15.223 | 1.00 39.60 |
| ATOM | 19205 | | LEU | 2868 | 57.701 | 10.724 | 15.682 | 1.00 40.79 |
| ATOM | 19206 | | LEU | 2868 | 56.167 | 10.790 | 13.709 | 1.00 40.12 |
| ATOM | 19207 | С | LEU | 2868 | 53.189 | 8.655 | 16.003 | 1.00 38.24 |
| MOTA | 19208 | 0 | LEU | 2868 | 52.981 | 7.817 | 15.124 | 1.00 37.72 |
| ATOM | 19209 | N | ALA | 2869 | 52.853 | 8.470 | 17.275 | 1.00 36.58 |
| ATOM | 19210 | CA | ALA | 2869 | 52.197 | 7.246 | 17.723 | 1.00 36.98 |
| ATOM | 19211 | СВ | ALA | 2869 | 52.156 | 7.206 | 19.245 | 1.00 36.32 |
| ATOM | 19212 | С | ALA | 2869 | 50.782 | 7.165 | 17.157 | 1.00 36.13 |
| MOTA | 19213 | 0 | ALA | 2869 | 50.346 | 6.109 | 16.699 | 1.00 37.03 |
| MOTA | 19214 | N | LEU | 2870 | 50.070 | 8.287 | 17.195 | 1.00 35.62 |
| MOTA | 19215 | CA | LEU | 2870 | 48.705 | 8.349 | 16.684 | 1.00 35.07 |
| MOTA | 19216 | CB | LEU | 2870 | 48.091 | 9.719 | 16.990 | 1.00 35.82 |
| MOTA | 19217 | CG | LEU | 2870 | 47.905 | 10.070 | 18.471 | 1.00 36.77 |
| MOTA | 19218 | CD1 | LEU | 2870 | 47.517 | 11.530 | 18.606 | 1.00 37.65 |
| MOTA | 19219 | CD2 | LEU | 2870 | 46.842 | 9.171 | 19.087 | 1.00 37.97 |
| MOTA | 19220 | С | LEU | 2870 | 48.703 | 8.099 | 15.180 | 1.00 33.74 |
| MOTA | 19221 | 0 | LEU | 2870 | 47.826 | 7.413 | 14.655 | 1.00 32.74 |
| MOTA | 19222 | N | GLU | 2871 | 49.692 | 8.656 | 14.489 | 1.00 33.03 |
| ATOM | 19223 | CA | GLU | 2871 | 49.807 | 8.480 | 13.047 | 1.00 31.65 |
| MOTA | 19224 | CB | GLU | 2871 | 50.952 | 9.338 | 12.501 | 1.00 32.99 |
| MOTA | 19225 | CG | GLU | 2871 | 51.193 | 9.165 | 11.011 | 1.00 33.67 |
| MOTA | 19226 | CD | GLU | 2871 | 52.375 | 9.974 | 10.518 | 1.00 34.78 |
| MOTA | 19227 | OE1 | GLU | 2871 | 53.477 | 9.806 | 11.085 | 1.00 33.73 |
| MOTA | 19228 | OE2 | GLU | 2871 · | 52.205 | 10.766 | 9.567 | 1.00 35.40 |
| MOTA | 19229 | С | GLU | 2871 | 50.061 | 7.015 | 12.715 | 1.00 31.63 |
| MOTA | 19230 | 0 | GLU | 2871 | 49.438 | 6.460 | 11.811 | 1.00 31.20 |
| MOTA | 19231 | N | ALA | 2872 | 50.975 | 6.391 | 13.451 | 1.00 30.57 |
| MOTA | 19232 | CA | ALA | 2872 | 51.306 | 4.988 | 13.221 | 1.00 30.98 |
| MOTA | 19233 | CB | ALA | 2872 | 52.506 | 4.588 | 14.076 | 1.00 30.03 |
| MOTA | 19234 | С | ALA | 2872 | 50.110 | 4.095 | 13.544 | 1.00 29.80 |
| MOTA | 19235 | 0 | ALA | 2872 | 49.949 | 3.020 | 12.965 | 1.00 28.80 |
| MOTA | 19236 | N | ALA | 2873 | 49.274 | 4.561 | 14.468 | 1.00 29.24 |
| MOTA | 19237 | CA | ALA | 2873 | 48.086 | 3.832 | 14.898 | 1.00 27.99 |
| MOTA | 19238 | CB | ALA | 2873 | 47.538 | 4.449 | 16.185 | 1.00 27.72 |
| MOTA | 19239 | С | ALA | 2873 | 47.010 | 3.825 | 13.818 | 1.00 28.11 |
| MOTA | 19240 | 0 | ALA | 2873 | 46.158 | 2.935 | 13.782 | 1.00 27.45 |
| ATOM | 19241 | N | GLY | 2874 | 47.044 | 4.821 | 12.939 | 1.00 26.89 |
| MOTA | 19242 | CA | GLY | 2874 | 46.059 | 4.883 | 11.874 | 1.00 27.96 |
| ATOM | 19243 | С | GLY | 2874 | 45.396 | 6.235 | 11.685 | 1.00 27.38 |
| MOTA | 19244 | 0 | GLY | 2874 | 44.639 | 6.428 | 10.736 | 1.00 27.45 |
| ATOM | 19245 | N | ALA | 2875 | 45.671 | 7.175 | 12.583 | 1.00 28.20 |
| ATOM | 19246 | CA | ALA | 2875 | 45.085 | 8.502 | 12.481 | 1.00 28.33 1.00 29.66 |
| ATOM | 19247 | СВ | ALA | 2875 | 45.556 | 9.366 | 13.640 | 1.00 29.00 |
| MOTA | 19248 | C | ALA | 2875 | 45.462 | 9.154 | 11.147 10.768 | 1.00 30.07 |
| ATOM | 19249 | O N | ALA | 2875 2876 | 46.634 44.466 | 9.176 9.679 | 10.786 | 1.00 30.07 |
| ATOM | 19250 19251 | N _. | GLN GLN | 2876 | 44.704 | 10.324 | 9.146 | 1.00 23.03 |
| MOTA MOTA | 19252 | CB | GLN | 2876 | 43.634 | 9.895 | 8.141 | 1.00 32.52 |
| ATOM | 19252 | CG | GLN | 2876 | 43.582 | 8.393 | 7.917 | |
| ATOM | 19254 | CD | GLN | 2876 | 42.514 | 7.983 | 6.922 | 1.00 35.64 |
| ATOM | 19255 | | GLN | 2876 | 42.635 | 8.238 | 5.720 | 1.00 37.92 |
| ATOM | 19256 | NE2 | | 2876 | 41.459 | 7.346 | 7.417 | 1.00 34.07 |
| ATOM | 19257 | C | GLN | 2876 | 44.716 | 11.842 | 9.270 | 1.00 32.63 |
| ATOM | 19258 | ō | GLN | 2876 | 44.871 | 12.556 | 8.278 | 1.00 32.11 |
| ATOM | 19259 | N | LEU | 2877 | 44.560 | 12.321 | 10.500 | 1.00 34.15 |
| ATOM | 19260 | CA | LEU | 2877 | 44.547 | 13.750 | 10.794 | 1.00 35.91 |
| ATOM | 19261 | CB | LEU | 2877 | 43.154 | 14.329 | 10.547 | 1.00 36.23 |
| ATOM | 19262 | CG | LEU | 2877 | 42.960 | 15.163 | 9.283 | 1.00 37.74 |
| ATOM | 19263 | | LEU | 2877 | 41.505 | 15.594 | 9.176 | 1.00 37.26 |
| ATOM | 19264 | CD2 | LEU | 2877 | 43.877 | 16.373 | 9.332 | 1.00 37.89 |
| ATOM | 19265 | С | LEU | 2877 | 44.933 | 13.990 | 12.244 | 1.00 36.30 |
| ATOM | 19266 | 0 | LEU | 2877 | 44.750 | 13.117 | 13.090 | 1.00 36.32 |
| MOTA | 19267 | N | LEU | 2878 | 45.465 | 15.178 | 12.522 | 1.00 37.48 |
| MOTA | 19268 | CA | LEU | 2878 | 45.875 | 15.555 | 13.873 | 1.00 38.35 |
| MOTA | 19269 | CB | LEU | 2878 | 47.379 | 15.346 | 14.057 | 1.00 37.59 |
| MOTA | 19270 | CG | LEU | 2878 | 47.944 | 15.762 | 15.418 | 1.00 38.15 |
| ATOM | 19271 | | LEU | 2878 | 47.332 | 14.906 | 16.517 | 1.00 37.53 |
| ATOM | 19272 | | LEU | 2878 | 49.458 | 15.611 | 15.411 | 1.00 38.68 |
| ATOM | 19273 | С | LEU | 2878 | 45.535 | 17.017 | 14.151 | 1.00 39.83 |
| ATOM | 19274 | 0 | LEU | 2878 | 45.609 | 17.861 | 13.257 | 1.00 39.08 |
| MOTA | 19275 | N | VAL | 2879 | 45.162 | 17.309 | 15.393 | 1.00 41.38 |
| MOTA | 19276 | CA | VAL | 2879 | 44.820 | 18.670 | 15.793 | 1.00 42.90 |
| MOTA | 19277 | CB | VAL | 2879 | 43.342 | 18.778 | 16.231 | 1.00 42.29 |
| MOTA | 19278 | CG1 | VAL | 2879 | 43.035 | 20.196 | 16.685 | 1.00 42.71 |

| ATOM | 19279 | CG2 | VAL | 2879 | 42.433 | 18.384 | 15.086 | 1.00 41.99 |
|------|-------|-----|-----|------|------------------|--------|------------------|------------|
| ATOM | 19280 | C | VAL | 2879 | 45.700 | 19.133 | 16.949 | 1.00 44.01 |
| ATOM | 19281 | ō | VAL | 2879 | 45.791 | 18.468 | 17.983 | 1.00 43.86 |
| ATOM | 19282 | N | LEU | 2880 | 46.352 | 20.276 | 16.760 | 1.00 45.45 |
| ATOM | 19283 | CA | LEU | 2880 | 47.221 | 20.852 | 17.781 | 1.00 47.07 |
| ATOM | 19284 | CB | LEU | 2880 | 48.564 | 21.261 | 17.170 | 1.00 47.30 |
| | | CG | LEU | 2880 | 49.446 | 20.136 | 16.632 | 1.00 47.79 |
| ATOM | 19285 | | | | | | 15.975 | |
| ATOM | 19286 | CD1 | | 2880 | 50.688 | 20.726 | | 1.00 48.71 |
| MOTA | 19287 | CD2 | | 2880 | 49.832 | 19.201 | 17.770 | 1.00 47.63 |
| MOTA | 19288 | С | LEU | 2880 | 46.539 | 22.073 | 18.381 | 1.00 48.19 |
| MOTA | 19289 | 0 | LEU | 2880 | 46.213 | 23.022 | 17.667 | 1.00 48.54 |
| MOTA | 19290 | N | GLU | 2881 | 46.326 | 22.047 | 19.692 | 1.00 49.26 |
| MOTA | 19291 | CA | GLU | 2881 | 45.668 | 23.154 | 20.377 | 1.00 51.27 |
| ATOM | 19292 | CB | GLU | 2881 | 44.478 | 22.635 | 21.186 | 1.00 51.11 |
| ATOM | 19293 | CG | GLU | 2881 | 43.547 | 23.724 | 21.684 | 1.00 52.03 |
| ATOM | 19294 | CD | GLU | 2881 | 42.497 | 23.196 | 22.631 | 1.00 51.94 |
| MOTA | 19295 | OE1 | GLU | 2881 | 41.810 | 22.220 | 22.271 | 1.00 51.97 |
| MOTA | 19296 | OE2 | GLU | 2881 | 42.358 | 23.756 | 23.740 | 1.00 53.44 |
| ATOM | 19297 | С | GLU | 2881 | 46.629 | 23.894 | 21.304 | 1.00 52.45 |
| ATOM | 19298 | 0 | GLU | 2881 | 47.177 | 23.308 | 22.239 | 1.00 51.90 |
| ATOM | 19299 | N | CYS | 2882 | 46.818 | 25.185 | 21.038 | 1.00 53.90 |
| MOTA | 19300 | CA | CYS | 2882 | 47.705 | 26.033 | 21.832 | 1.00 55.11 |
| ATOM | 19301 | CB | CYS | 2882 | 47.038 | 26.398 | 23.159 | 1.00 55.59 |
| ATOM | 19302 | SG | CYS | 2882 | 45.596 | 27.473 | 22.965 | 1.00 57.79 |
| MOTA | 19302 | C | CYS | 2882 | 49.054 | 25.381 | 22.095 | 1.00 55.25 |
| ATOM | 19304 | o | CYS | 2882 | 49.260 | 24.729 | 23.119 | 1.00 55.61 |
| | | | | 2883 | 49.974 | 25.570 | 21.158 | 1.00 55.88 |
| ATOM | 19305 | N | VAL | | | | | 1.00 56.54 |
| ATOM | 19306 | CA | VAL | 2883 | 51.312 | 25.006 | 21.264 20.601 | |
| ATOM | 19307 | CB | VAL | 2883 | 51.364 | 23.606 | | 1.00 56.77 |
| MOTA | 19308 | | VAL | 2883 | 50.923 | 23.700 | 19.150 | 1.00 57.14 |
| MOTA | 19309 | | VAL | 2883 | 52.764 | 23.029 | 20.694 | 1.00 56.92 |
| MOTA | 19310 | С | VAL | 2883 | 52.291 | 25.949 | 20.568 | 1.00 56.70 |
| MOTA | 19311 | 0 | VAL | 2883 | 51.988 | 26.489 | 19.502 | 1.00 56.49 |
| MOTA | 19312 | N | PRO | 2884 | 53.476 | 26.168 | 21.167 | 1.00 56.87 |
| MOTA | 19313 | CD | PRO | 2884 | 54.038 | 25.483 | 22.342 | 1.00 56.82 |
| MOTA | 19314 | CA | PRO | 2884 | 54.473 | 27.060 | 20.565 | 1.00 56.93 |
| MOTA | 19315 | CB | PRO | 2884 | 55.699 | 26.863 | 21.459 | 1.00 56.72 |
| MOTA | 19316 | CG | PRO | 2884 | 55.503 | 25.482 | 22.019 | 1.00 57.13 |
| ATOM | 19317 | С | PRO | 2884 | 54.747 | 26.718 | 19.105 | 1.00 57.27 |
| MOTA | 19318 | 0 | PRO | 2884 | 54.999 | 25.562 | 18.766 | 1.00 57.23 |
| MOTA | 19319 | N | VAL | 2885 | 54.689 | 27.735 | 18.250 | 1.00 56.98 |
| ATOM | 19320 | CA | VAL | 2885 | 54.908 | 27.564 | 16.818 | 1.00 57.68 |
| ATOM | 19321 | СВ | VAL | 2885 | 55.176 | 28.918 | 16.129 | 1.00 57.41 |
| ATOM | 19322 | CG1 | VAL | 2885 | 55.141 | 28.747 | 14.620 | 1.00 57.11 |
| ATOM | 19323 | CG2 | VAL | 2885 | 54.150 | 29.942 | 16.578 | 1.00 57.26 |
| ATOM | 19324 | C | VAL | 2885 | 56.079 | 26.632 | 16.519 | 1.00 58.32 |
| ATOM | 19325 | ō | VAL | 2885 | 56.046 | 25.867 | 15.553 | 1.00 58.54 |
| ATOM | 19326 | N | GLU | 2886 | 57.108 | 26.701 | 17.358 | 1.00 58.72 |
| ATOM | 19327 | CA | GLU | 2886 | 58.300 | 25.876 | 17.194 | 1.00 58.51 |
| ATOM | 19328 | СВ | GLU | 2886 | 59.282 | 26.138 | 18.341 | 1.00 59.10 |
| MOTA | 19329 | CG | GLU | 2886 | 59.379 | 27.602 | 18.763 | 1.00 59.54 |
| MOTA | 19330 | CD | GLU | 2886 | 59.529 | 28.549 | 17.586 | |
| | 19331 | | GLU | 2886 | | 28.357 | 16.779 | 1.00 60.96 |
| ATOM | | OE2 | | | 60.465 58.711 | 29.488 | 17.473 | 1.00 59.20 |
| MOTA | 19332 | | | 2886 | 57.937 | | 17.164 | 1.00 58.20 |
| MOTA | 19333 | С | GLU | 2886 | | 24.394 | | |
| MOTA | 19334 | 0 | GLU | 2886 | 58.373 | 23.650 | 16.283 | 1.00 57.63 |
| ATOM | 19335 | N | LEU | 2887 | 57.131 | 23.975 | 18.134 | 1.00 57.62 |
| MOTA | 19336 | CA | LEU | 2887 | 56.706 | 22.586 | 18.235 | 1.00 57.41 |
| MOTA | 19337 | СВ | LEU | 2887 | 55.937 | 22.371 | 19.540 | 1.00 56.08 |
| MOTA | 19338 | CG | LEU | 2887 | 56.331 | 21.145 | 20.368 | 1.00 55.97 |
| MOTA | 19339 | | LEU | 2887 | 55.545 | 21.140 | 21.668 | 1.00 55.92 |
| MOTA | 19340 | CD2 | LEU | 2887 | 56.075 | 19.875 | 19.578 | 1.00 55.54 |
| MOTA | 19341 | С | LEU | 2887 | 55.833 | 22.193 | 17.046 | 1.00 57.47 |
| MOTA | 19342 | 0 | LEU | 2887 | 55.948 | 21.086 | 16.519 | 1.00 57.79 |
| MOTA | 19343 | N | ALA | 2888 | 54.962 | 23.106 | 16.628 | 1.00 57.65 |
| MOTA | 19344 | CA | ALA | 2888 | 54.071 | 22.861 | 15.500 | 1.00 57.47 |
| MOTA | 19345 | СВ | ALA | 2888 | 53.138 | 24.051 | | 1.00 57.84 |
| ATOM | 19346 | С | ALA | 2888 | 54.859 | 22.604 | 14.219 | 1.00 57.89 |
| ATOM | 19347 | 0 | ALA | 2888 | 54.491 | 21.751 | 13.411 | 1.00 57.53 |
| MOTA | 19348 | N | LYS | 2889 | 55.944 | 23.352 | 14.040 | 1.00 57.61 |
| MOTA | 19349 | CA | LYS | 2889 | 56.790 | 23.211 | 12.862 | 1.00 57.71 |
| ATOM | 19350 | СВ | LYS | 2889 | 57.952 | 24.205 | 12.929 | 1.00 58.61 |
| MOTA | 19351 | CG | LYS | 2889 | 57.518 | 25.662 | 12.982 | 1.00 60.67 |
| MOTA | 19352 | CD | LYS | 2889 | 58.694 | 26.590 | 13.263 | 1.00 62.37 |
| ATOM | 19353 | CE | LYS | 2889 | 58.243 | 28.043 | 13.347 | 1.00 62.84 |
| ATOM | 19354 | NZ | LYS | 2889 | 59.353 | 28.959 | 13.729 | 1.00 63.21 |
| ATOM | 19355 | C | LYS | 2889 | 57.337 | 21.794 | 12.763 | 1.00 57.10 |
| | | - | | | 2 | | | |

| ATOM | 19356 | 0 | LYS | 2889 | 57.302 | 21.180 | 11.696 | 1.00 57.17 |
|-------|-------|-----|-------------|------|--------|--------|--------|------------|
| | 19357 | N | ARG | 2890 | 57.840 | 21.281 | 13.881 | 1.00 56.24 |
| MOTA | | | | | | | | |
| MOTA | 19358 | CA | ARG | 2890 | 58.401 | 19.936 | 13.923 | 1.00 55.63 |
| MOTA | 19359 | CB | ARG | 2890 | 58.973 | 19.639 | 15.311 | 1.00 56.65 |
| ATOM | 19360 | CG | ARG | 2890 | 60.157 | 20.501 | 15.697 | 1.00 58.26 |
| ATOM | 19361 | CD | ARG | 2890 | 60.844 | 19.945 | 16.934 | 1.00 60.00 |
| | | | | | 59.947 | 19.894 | 18.084 | 1.00 61.53 |
| MOTA | 19362 | NE | ARG | 2890 | | | | |
| MOTA | 19363 | CZ | ARG | 2890 | 60.260 | 19.344 | 19.254 | 1.00 62.29 |
| MOTA | 19364 | NH1 | ARG | 2890 | 61.451 | 18.791 | 19.433 | 1.00 62.17 |
| ATOM | 19365 | NH2 | ARG | 2890 | 59.381 | 19.349 | 20.246 | 1.00 63.05 |
| | 19366 | C | ARG | 2890 | 57.364 | 18.880 | 13.573 | 1.00 54.19 |
| MOTA | | | | | | | | |
| MOTA | 19367 | 0 | ARG | 2890 | 57.502 | 18.162 | 12.584 | 1.00 53.84 |
| MOTA | 19368 | N | ILE | 2891 | 56.329 | 18.790 | 14.401 | 1.00 52.97 |
| MOTA | 19369 | CA | ILE | 2891 | 55.256 | 17.826 | 14.202 | 1.00 51.09 |
| MOTA | 19370 | CB | ILE | 2891 | 54.099 | 18.088 | 15.187 | 1.00 51.37 |
| MOTA | 19371 | CG2 | ILE | 2891 | 52.970 | 17.095 | 14.947 | 1.00 50.95 |
| | | | | | | | | |
| MOTA | 19372 | CG1 | ILE | 2891 | 54.613 | 17.981 | 16.626 | 1.00 50.98 |
| MOTA | 19373 | CD1 | ILE | 2891 | 53.598 | 18.382 | 17.676 | 1.00 50.45 |
| MOTA | 19374 | С | ILE | 2891 | 54.712 | 17.874 | 12.777 | 1.00 50.48 |
| ATOM | 19375 | 0 | ILE | 2891 | 54.621 | 16.845 | 12.108 | 1.00 50.45 |
| | 19376 | | | 2892 | 54.358 | 19.069 | 12.316 | 1.00 49.45 |
| ATOM | | N | THR | | | | | |
| MOTA | 19377 | CA | THR | 2892 | 53.816 | 19.230 | 10.973 | 1.00 49.23 |
| MOTA | 19378 | CB | THR | 2892 | 53.557 | 20.713 | 10.637 | 1.00 48.82 |
| ATOM | 19379 | OG1 | THR | 2892 | 52.662 | 21.275 | 11.603 | 1.00 49.13 |
| ATOM | 19380 | CG2 | THR | 2892 | 52.937 | 20.843 | 9.249 | 1.00 48.85 |
| | | | | | | | 9.908 | 1.00 49.30 |
| ATOM | 19381 | C | THR | 2892 | 54.740 | 18.649 | | |
| MOTA | 19382 | 0 | THR | 2892 | 54.280 | 18.005 | 8.965 | 1.00 48.82 |
| ATOM | 19383 | N | GLU | 2893 | 56.041 | 18.878 | 10.056 | 1.00 49.78 |
| MOTA | 19384 | CA | GLU | 2893 | 57.007 | 18.369 | 9.088 | 1.00 50.32 |
| | 19385 | CB | GLU | 2893 | 58.245 | 19.268 | 9.043 | 1.00 51.93 |
| ATOM | | | | | | | | |
| ATOM | 19386 | CG | GLU | 2893 | 57.979 | 20.650 | 8.460 | 1.00 54.14 |
| MOTA | 19387 | CD | GLU | 2893 | 59.255 | 21.412 | 8.163 | 1.00 55.53 |
| MOTA | 19388 | OE1 | GLU | 2893 | 60.036 | 21.666 | 9.106 | 1.00 55.46 |
| ATOM | 19389 | OE2 | GLU | 2893 | 59.477 | 21.757 | 6.982 | 1.00 56.24 |
| | | | | | | 16.933 | 9.381 | 1.00 49.42 |
| MOTA | 19390 | С | GLU | 2893 | 57.423 | | | |
| MOTA | 19391 | 0 | GLU | 2893 | 57.953 | 16.243 | 8.509 | 1.00 49.42 |
| ATOM | 19392 | N | ALA | 2894 | 57.174 | 16.487 | 10.609 | 1.00 48.11 |
| MOTA | 19393 | CA | ALA | 2894 | 57.518 | 15.131 | 11.021 | 1.00 46.74 |
| ATOM | 19394 | СВ | ALA | 2894 | 57.718 | 15.079 | 12.531 | 1.00 46.75 |
| | | | | | | | | |
| MOTA | 19395 | С | ALA | 2894 | 56.438 | 14.135 | 10.604 | 1.00 45.44 |
| MOTA | 19396 | 0 | ALA | 2894 | 56.721 | 12.959 | 10.379 | 1.00 45.28 |
| MOTA | 19397 | N | LEU | 2895 | 55.200 | 14.608 | 10.500 | 1.00 44.09 |
| ATOM | 19398 | CA | LEU | 2895 | 54.097 | 13.740 | 10.112 | 1.00 42.66 |
| ATOM | 19399 | CB | LEU | 2895 | 52.845 | 14.067 | 10.932 | 1.00 43.61 |
| | | | | | | | 12.450 | 1.00 43.86 |
| MOTA | 19400 | CG | LEU | 2895 | 52.966 | 13.940 | | |
| MOTA | 19401 | | LEU | 2895 | 51.651 | 14.323 | 13.105 | 1.00 44.30 |
| MOTA | 19402 | CD2 | LEU | 2895 | 53.350 | 12.520 | 12.814 | 1.00 45.06 |
| MOTA | 19403 | С | LEU | 2895 | 53.777 | 13.884 | 8.631 | 1.00 41.50 |
| MOTA | 19404 | 0 | LEU | 2895 | 53.887 | 14.973 | 8.067 | 1.00 41.74 |
| ATOM | 19405 | N | ALA | 2896 | 53.384 | 12.776 | 8.009 | 1.00 39.31 |
| | | | | | | | | |
| ATOM | 19406 | CA | ALA | 2896 | 53.020 | 12.769 | 6.597 | 1.00 37.81 |
| MOTA | 19407 | CB | ALA | 2896 | 53.230 | 11.380 | 6.003 | 1.00 37.19 |
| MOTA | 19408 | С | ALA | 2896 | 51.558 | 13.178 | 6.468 | 1.00 37.41 |
| ATOM. | 19409 | 0 | ALA · | 2896 | 51.144 | 13.749 | 5.458 | 1.00 35.35 |
| ATOM | 19410 | N | ILE | 2897 | 50.776 | 12.874 | 7.499 | 1.00 37.72 |
| | | | | | | | | |
| | 19411 | CA | ILE | 2897 | 49.359 | 13.222 | 7.510 | 1.00 37.82 |
| MOTA | 19412 | CB | $_{ m ILE}$ | 2897 | 48.589 | 12.404 | 8.572 | 1.00 38.19 |
| MOTA | 19413 | CG2 | ILE | 2897 | 48.562 | 10.938 | 8.182 | 1.00 35.52 |
| ATOM | 19414 | CG1 | ILE | 2897 | 49.237 | 12.602 | 9.947 | 1.00 36.77 |
| MOTA | 19415 | CD1 | ILE | 2897 | 48.490 | 11.937 | 11.083 | 1.00 38.83 |
| | | | | | | | | |
| MOTA | 19416 | C | ILE | 2897 | 49.202 | 14.706 | 7.825 | 1.00 38.40 |
| ATOM | 19417 | 0 | ILE | 2897 | 49.987 | 15.274 | 8.585 | 1.00 37.92 |
| MOTA | 19418 | N | PRO | 2898 | 48.180 | 15.354 | 7.247 | 1.00 38.51 |
| MOTA | 19419 | CD | PRO | 2898 | 47.116 | 14.796 | 6.397 | 1.00 38.81 |
| ATOM | 19420 | CA | PRO | 2898 | 47.953 | 16.781 | 7.492 | 1.00 39.39 |
| ATOM | 19421 | CB | PRO | 2898 | 46.729 | 17.090 | 6.629 | 1.00 39.31 |
| | | | | | | | | |
| ATOM | 19422 | CG | PRO | 2898 | 46.001 | 15.787 | 6.601 | 1.00 40.01 |
| MOTA | 19423 | С | PRO | 2898 | 47.730 | 17.097 | 8.968 | 1.00 40.59 |
| MOTA | 19424 | 0 | PRO | 2898 | 46.998 | 16.391 | 9.665 | 1.00 40.56 |
| MOTA | 19425 | N | VAL | 2899 | 48.375 | 18.158 | 9.441 | 1.00 40.40 |
| ATOM | 19426 | CA | VAL | 2899 | 48.252 | 18.569 | 10.832 | 1.00 40.89 |
| | | | | | | | | |
| ATOM | 19427 | CB | VAL | 2899 | 49.641 | 18.739 | 11.484 | 1.00 41.08 |
| MOTA | 19428 | | VAL | 2899 | 49.487 | 19.099 | 12.952 | 1.00 40.58 |
| MOTA | 19429 | CG2 | VAL | 2899 | 50.442 | 17.457 | 11.334 | 1.00 41.04 |
| ATOM | 19430 | С | VAL | 2899 | 47.489 | 19.882 | 10.942 | 1.00 41.61 |
| ATOM | 19431 | ō | VAL | 2899 | 48.002 | 20.946 | 10.594 | 1.00 42.66 |
| ATOM | 19432 | N | | | 46.254 | 19.797 | 11.424 | 1.00 41.85 |
| AIOM | 19434 | 1.4 | ILE | 2900 | 40.234 | 17.191 | 11.424 | T.00 4T.03 |
| | | | | | | | | |

| ATOM | 19433 | CA | ILE | 2900 | 45.409 | 20.973 | 11.588 | 1.00 40.80 |
|--------------|----------------|------------|------------|--------------|------------------|------------------|------------------|--------------------------|
| MOTA | 19434 | CB | ILE | 2900 | 43.918 | 20.589 | 11.510 | 1.00 40.42 |
| MOTA | 19435 | CG2 | ILE | 2900 | 43.046 | 21.818 | 11.739 | 1.00 40.48 |
| MOTA | 19436 | CG1 | ILE | 2900 | 43.627 | 19.954 | 10.146 | 1.00 40.12 |
| ATOM | 19437 | CD1 | ILE | 2900 | 42.223 | 19.401 | 10.000 | 1.00 38.79 |
| MOTA | 19438 | С | ILE | 2900 | 45.701 | 21.599 | 12.943 | 1.00 40.37 |
| MOTA | 19439 | 0 | ILE | 2900 | 45.760 | 20.902 | 13.955 | 1.00 40.86 |
| MOTA | 19440 | N | GLY | 2901 | 45.892 | 22.913 | 12.964 | 1.00 40.33 |
| MOTA | 19441 | CA | GLY | 2901 | 46.189 | 23.576 | 14.219 | 1.00 39.83 1.00 39.82 |
| ATOM | 19442 | C | GLY | 2901 2901 | 45.312 44.743 | 24.771 25.400 | 14.534 13.644 | 1.00 39.82 |
| ATOM ATOM | 19443 19444 | O N | GLY ILE | 2902 | 45.198 | 25.400 | 15.822 | 1.00 40.24 |
| ATOM | 19445 | CA | ILE | 2902 | 44.414 | 26.203 | 16.287 | 1.00 41.59 |
| ATOM | 19446 | СВ | ILE | 2902 | 43.043 | 25.758 | 16.859 | 1.00 41.56 |
| MOTA | 19447 | CG2 | ILE | 2902 | 43.232 | 24.634 | 17.871 | 1.00 39.96 |
| MOTA | 19448 | CG1 | ILE | 2902 | 42.333 | 26.957 | 17.490 | 1.00 42.23 |
| MOTA | 19449 | CD1 | ILE | 2902 | 40.886 | 26.696 | 17.857 | 1.00 42.44 |
| MOTA | 19450 | С | ILE | 2902 | 45.225 | 26.913 | 17.364 | 1.00 42.95 |
| MOTA | 19451 | 0 | ILE | 2902 | 45.405 | 26.397 | 18.468 | 1.00 41.71 |
| ATOM | 19452 | N | GLY | 2903 | 45.729 | 28.096 | 17.027 | 1.00 44.58 |
| MOTA | 19453 | CA | GLY | 2903 | 46.535 | 28.845 | 17.972 | 1.00 45.63 |
| ATOM | 19454 | C | GLY | 2903 | 47.918 | 28.234 | 18.068 | 1.00 46.17 |
| MOTA | 19455 19456 | O N | GLY | 2903 2904 | 48.531 48.407 | 28.218 27.722 | 19.136 16.942 | 1.00 46.79 1.00 46.61 |
| ATOM ATOM | 19457 | N CA | ALA ALA | 2904 | 49.725 | 27.122 | 16.887 | 1.00 46.93 |
| ATOM | 19458 | CB | ALA | 2904 | 49.584 | 25.594 | 16.723 | 1.00 46.40 |
| ATOM | 19459 | C | ALA | 2904 | 50.565 | 27.674 | 15.749 | 1.00 46.66 |
| ATOM | 19460 | ō | ALA | 2904 | 51.652 | 27.174 | 15.461 | 1.00 46.67 |
| ATOM | 19461 | N | GLY | 2905 | 50.056 | 28.718 | 15.100 | 1.00 47.11 |
| ATOM | 19462 | CA | GLY | 2905 | 50.786 | 29.331 | 14.004 | 1.00 47.45 |
| MOTA | 19463 | C | GLY | 2905 | 50.290 | 28.905 | 12.634 | 1.00 48.01 |
| MOTA | 19464 | 0 | GLY | 2905 | 49.434 | 28.027 | 12.517 | 1.00 48.29 |
| MOTA | 19465 | N | ASN | 2906 | 50.832 | 29.528 | 11.591 | 1.00 47.47 |
| ATOM | 19466 | CA | ASN | 2906 | 50.439 | 29.213 | 10.221 | 1.00 47.27 |
| ATOM | 19467 | CB | ASN | 2906 | 50.423 | 30.488 | 9.373 9.346 | 1.00 46.79 |
| ATOM | 19468 19469 | CG OD1 | ASN ASN | 2906 2906 | 51.771 51.940 | 31.187 32.206 | 8.674 | 1.00 46.39 |
| ATOM ATOM | 19470 | | ASN | 2906 | 52.736 | 30.644 | 10.079 | 1.00 47.13 |
| ATOM | 19471 | C | ASN | 2906 | 51.374 | 28.190 | 9.585 | 1.00 47.11 |
| MOTA | 19472 | ō | ASN | 2906 | 51.368 | 28.002 | 8.366 | 1.00 46.64 |
| ATOM | 19473 | N | VAL | 2907 | 52.173 | 27.530 | 10.418 | 1.00 47.09 |
| MOTA | 19474 | CA | VAL | 2907 | 53.118 | 26.526 | 9.941 | 1.00 47.56 |
| MOTA | 19475 | CB | VAL | 2907 | 54.234 | 26.269 | 10.980 | 1.00 48.05 |
| MOTA | 19476 | | VAL | 2907 | 55.286 | 25.336 | 10.394 | 1.00 49.38 |
| MOTA | 19477 | CG2 | VAL | 2907 | 54.866 | 27.584 | 11.404 | 1.00 48.66 |
| MOTA | 19478 | C | VAL | 2907 | 52.415 | 25.204 | 9.645 | 1.00 47.40 |
| ATOM | 19479 | 0 | VAL | 2907 | 52.875 51.299 | 24.419 | 8.816 | 1.00 46.82 |
| ATOM ATOM | 19480 19481 | N CA | THR THR | 2908 2908 | 50.538 | 24.965 23.737 | 10.326 10.134 | 1.00 46.84 1.00 46.83 |
| ATOM | 19482 | CB | THR | 2908 | 49.387 | 23.644 | 11.145 | 1.00 46.34 |
| ATOM | 19483 | OG1 | | 2908 | 48.608 | 24.845 | 11.091 | 1.00 47.58 |
| ATOM | 19484 | | THR | 2908 | 49.932 | 23.460 | 12.550 | 1.00 45.22 |
| MOTA | 19485 | С | THR | 2908 | 49.966 | 23.646 | 8.722 | 1.00 47.30 |
| ATOM | 19486 | 0 | THR | 2908 | 49.862 | 24.649 | 8.013 | 1.00 47.83 |
| MOTA | 19487 | N | ASP | 2909 | 49.598 | 22.436 | 8.318 | 1.00 46.81 |
| MOTA | 19488 | CA | ASP | 2909 | 49.047 | 22.204 | 6.989 | 1.00 47.02 |
| MOTA | 19489 | CB | ASP | 2909 | 48.974 | 20.700 | 6.718 | 1.00 47.68 |
| MOTA | 19490 | CG | ASP | 2909 | 50.313 | 20.009 | 6.906 | |
| MOTA | 19491 | | ASP | 2909 2909 | 51.248 50.432 | 20.299 19.182 | 6.127 7.836 | 1.00 49.06 1.00 47.98 |
| MOTA MOTA | 19492 19493 | C C | ASP ASP | 2909 | 47.666 | 22.831 | 6.832 | 1.00 47.38 |
| ATOM | 19494 | o | ASP | 2909 | 47.219 | 23.110 | 5.717 | 1.00 46.70 |
| MOTA | 19495 | N | GLY | 2910 | 46.995 | 23.057 | 7.956 | 1.00 46.85 |
| ATOM | 19496 | CA | GLY | 2910 | 45.672 | 23.650 | 7.914 | 1.00 46.10 |
| ATOM | 19497 | С | GLY | 2910 | 45.335 | 24.437 | 9.163 | 1.00 45.53 |
| MOTA | 19498 | 0 | GLY | 2910 | 46.113 | 24.473 | 10.115 | 1.00 44.71 |
| MOTA | 19499 | N | GLN | 2911 | 44.166 | 25.067 | 9.157 | 1.00 45.89 |
| ATOM | 19500 | CA | GLN | 2911 | 43.712 | 25.863 | 10.292 | 1.00 46.51 |
| ATOM | 19501 | CB | GLN | 2911 | 43.873 | 27.357 | 9.990 | 1.00 46.39 |
| MOTA | 19502 | CG | GLN | 2911 | 45.315 | 27.843 | 9.878 | 1.00 44.82 |
| ATOM | 19503 | CD OF1 | GLN | 2911 | 46.100 45.634 | 27.649 27.997 | 11.162 12.246 | 1.00 44.00 1.00 43.65 |
| MOTA MOTA | 19504 19505 | OE1 NE2 | GLN GLN | 2911 2911 | 45.634 | 27.997 | 12.246 | 1.00 43.65 |
| ATOM | 19506 | NE2 | GLN. | 2911 | 42.250 | 25.577 | 10.619 | 1.00 47.63 |
| ATOM | 19507 | 0 | GLN. | 2911 | 41.487 | 25.114 | 9.771 | 1.00 46.88 |
| ATOM | 19508 | N | ILE | 2912 | 41.867 | 25.853 | 11.860 | 1.00 48.52 |
| MOTA | 19509 | CA | ILE | 2912 | 40.492 | 25.652 | 12.290 | 1.00 50.21 |
| | | | | | | | | |

| ATOM | 19510 | CB | ILE | 2912 | 40.320 | 24.298 | 13.023 | 1.00 50.95 |
|------|--------|-----|-----|------|--------|--------|--------|------------|
| ATOM | 19511 | CG2 | ILE | 2912 | 41.195 | 24.257 | 14.270 | 1.00 51.75 |
| ATOM | 19512 | CG1 | ILE | 2912 | 38.849 | 24.088 | 13.376 | 1.00 51.34 |
| | | CD1 | ILE | 2912 | 38.484 | 22.641 | 13.645 | 1.00 52.84 |
| ATOM | 19513 | | | | | | | 1.00 50.85 |
| MOTA | 19514 | С | ILE | 2912 | 40.093 | 26.806 | 13.205 | |
| MOTA | 19515 | 0 | ILE | 2912 | 40.870 | 27.222 | 14.066 | 1.00 51.15 |
| MOTA | 19516 | N | LEU | 2913 | 38.889 | 27.334 | 13.005 | 1.00 51.43 |
| ATOM | 19517 | CA | LEU | 2913 | 38.417 | 28.456 | 13.808 | 1.00 51.62 |
| ATOM | 19518 | CB | LEU | 2913 | 38.566 | 29.760 | 13.012 | 1.00 52.42 |
| ATOM | 19519 | CG | LEU | 2913 | 39.031 | 31.024 | 13.747 | 1.00 53.65 |
| ATOM | 19520 | | LEU | 2913 | 39.235 | 32.140 | 12.739 | 1.00 53.91 |
| | | | | 2913 | 38.016 | | 14.802 | 1.00 54.69 |
| ATOM | 19521 | CD2 | LEU | | | 31.436 | | |
| MOTA | 19522 | С | LEU | 2913 | 36.964 | 28.277 | 14.240 | 1.00 50.63 |
| MOTA | 19523 | 0 | LEU | 2913 | 36.170 | 27.629 | 13.553 | 1.00 50.30 |
| ATOM | 19524 | N | VAL | 2914 | 36.627 | 28.853 | 15.389 | 1.00 49.32 |
| MOTA | 19525 | CA | VAL | 2914 | 35.274 | 28.778 | 15.922 | 1.00 47.68 |
| MOTA | 19526 | CB | VAL | 2914 | 35.275 | 28.908 | 17.455 | 1.00 48.06 |
| ATOM | 19527 | CG1 | VAL | 2914 | 33.877 | 28.658 | 18.003 | 1.00 49.28 |
| ATOM | 19528 | | VAL | 2914 | 36.268 | 27.930 | 18.050 | 1.00 47.75 |
| ATOM | 19529 | C | VAL | 2914 | 34.463 | 29.920 | 15.324 | 1.00 46.26 |
| | | | | 2914 | 34.721 | 31.092 | 15.601 | 1.00 45.66 |
| ATOM | 19530 | 0 | VAL | | | | | |
| MOTA | 19531 | N | MET | 2915 | 33.486 | | 14.496 | 1.00 43.97 |
| MOTA | 19532 | CA | MET | 2915 | 32.649 | 30.563 | 13.839 | 1.00 42.92 |
| MOTA | 19533 | CB | MET | 2915 | 31.500 | 29.873 | 13.106 | 1.00 40.64 |
| MOTA | 19534 | CG | MET | 2915 | 30.616 | 29.023 | 14.000 | 1.00 38.03 |
| MOTA | 19535 | SD | MET | 2915 | 28.938 | 28.996 | 13.368 | 1.00 33.08 |
| MOTA | 19536 | CE | MET | 2915 | 28.260 | 30.449 | 14.185 | 1.00 34.77 |
| ATOM | 19537 | C | MET | 2915 | 32.087 | | 14.813 | 1.00 42.94 |
| | 19538 | ō | MET | 2915 | 31.937 | 32.766 | 14.468 | 1.00 43.50 |
| ATOM | | | | | | | | |
| ATOM | 19539 | N | HIS | 2916 | 31.778 | | 16.028 | 1.00 43.84 |
| MOTA | 19540 | CA | HIS | 2916 | 31.228 | | 17.047 | 1.00 43.99 |
| MOTA | 19541 | CB | HIS | 2916 | 30.839 | 31.221 | 18.279 | 1.00 43.48 |
| MOTA | 19542 | CG | HIS | 2916 | 29.606 | 30.396 | 18.080 | 1.00 42.85 |
| MOTA | 19543 | CD2 | HIS | 2916 | 29.446 | 29.097 | 17.733 | 1.00 42.66 |
| ATOM | 19544 | ND1 | HIS | 2916 | 28.336 | 30.925 | 18.176 | 1.00 42.76 |
| ATOM | 19545 | | HIS | 2916 | 27.448 | | 17.897 | 1.00 42.12 |
| ATOM | 19546 | NE2 | HIS | 2916 | 28.095 | | 17.624 | 1.00 42.80 |
| | | | | | | | | 1.00 45.02 |
| MOTA | 19547 | С | HIS | 2916 | 32.192 | | 17.424 | |
| ATOM | 19548 | 0 | HIS | 2916 | 31.772 | | 17.871 | 1.00 43.97 |
| MOTA | 19549 | N | ASP | 2917 | 33.485 | | 17.238 | 1.00 46.22 |
| MOTA | 19550 | CA | ASP | 2917 | 34.493 | | 17.539 | 1.00 47.60 |
| MOTA | 19551 | CB | ASP | 2917 | 35.702 | 33.296 | 18.227 | 1.00 48.54 |
| MOTA | 19552 | CG | ASP | 2917 | 35.463 | 33.045 | 19.699 | 1.00 49.88 |
| ATOM | 19553 | OD1 | ASP | 2917 | 35.083 | 34.002 | 20.404 | 1.00 51.64 |
| ATOM | 19554 | | ASP | 2917 | 35.658 | | 20.156 | 1.00 51.53 |
| ATOM | 19555 | C | ASP | 2917 | 34.938 | | 16.266 | 1.00 47.64 |
| | | | | 2917 | 35.581 | | 16.317 | 1.00 49.23 |
| MOTA | 19556 | 0 | ASP | | | | | |
| ATOM | 19557 | N | ALA | 2918 | 34.587 | | 15.123 | 1.00 47.15 |
| MOTA | 19558 | CA | ALA | 2918 | 34.944 | | 13.833 | 1.00 46.36 |
| MOTA | 19559 | CB | ALA | 2918 | 34.938 | | 12.764 | 1.00 45.96 |
| MOTA | 19560 | С | ALA | 2918 | 33.965 | 35.736 | 13.463 | 1.00 46.60 |
| ATOM | 19561 | 0 | ALA | 2918 | 34.275 | 36.607 | | 1.00 45.86 |
| MOTA | 19562 | N | PHE | 2919 | 32.780 | 35.696 | 14.063 | 1.00 45.95 |
| ATOM | 19563 | CA | PHE | 2919 | 31.762 | | 13.794 | 1.00 46.21 |
| ATOM | 19564 | СВ | PHE | 2919 | 30.492 | | 13.274 | 1.00 47.19 |
| ATOM | 19565 | CG | PHE | 2919 | 30.738 | | 12.157 | 1.00 48.64 |
| ATOM | 19566 | | PHE | 2919 | 31.476 | | 11.038 | 1.00 49.33 |
| | | | | | 30.224 | | 12.219 | 1.00 49.14 |
| ATOM | 19567 | | PHE | 2919 | | | | |
| ATOM | 19568 | | PHE | 2919 | 31.698 | | 9.996 | 1.00 49.77 |
| ATOM | 19569 | CE2 | | 2919 | 30.440 | | 11.183 | 1.00 49.47 |
| ATOM | 19570 | CZ | PHE | 2919 | 31.177 | | 10.070 | 1.00 49.73 |
| ATOM | 19571 | С | PHE | 2919 | 31.450 | | 15.051 | 1.00 45.77 |
| ATOM | 19572 | 0 | PHE | 2919 | 30.435 | 38.193 | 15.122 | 1.00 45.54 |
| ATOM | 19573 | N | GLY | 2920 | 32.332 | 37.394 | 16.041 | 1.00 45.81 |
| ATOM | 19574 | CA | GLY | 2920 | 32.142 | | 17.289 | 1.00 46.37 |
| ATOM | 19575 | C | GLY | 2920 | 30.782 | | 17.909 | 1.00 46.48 |
| ATOM | 19576 | o | GLY | 2920 | 30.207 | | 18.530 | 1.00 45.85 |
| | | | | | 30.268 | | 17.741 | 1.00 46.20 |
| ATOM | 19577 | N | ILE | 2921 | | | | |
| ATOM | 19578 | CA | ILE | 2921 | 28.965 | | 18.286 | 1.00 47.25 |
| MOTA | 19579 | CB | ILE | 2921 | 28.450 | | 17.665 | 1.00 46.36 |
| ATOM | 19580 | CG2 | ILE | 2921 | 27.066 | | 18.210 | 1.00 46.13 |
| MOTA | 19581 | CG1 | ILE | 2921 | 28.410 | | 16.140 | 1.00 46.06 |
| ATOM | 19582 | CD1 | ILE | 2921 | 28.049 | 33.815 | 15.420 | 1.00 45.17 |
| ATOM | 19583 | С | ILE | 2921 | 29.040 | 36.120 | 19.801 | 1.00 48.32 |
| ATOM | 19584. | 0 | ILE | 2921 | 28.137 | | 20.526 | 1.00 47.30 |
| ATOM | 19585 | N. | | 2922 | 30.126 | | 20.271 | 1.00 50.35 |
| MOTA | 19586 | CA | THR | 2922 | 30.316 | | 21.696 | 1.00 53.99 |
| | | | | | 55.510 | 20.203 | | |
| | | | | | | | | |

| ATOM | 19587 | СВ | THR | 2922 | 31.599 | 34.487 | 21.960 | 1.00 53.75 |
|------|-------|-----|------|-------|--------|--------|--------|------------|
| ATOM | 19588 | OG1 | THR | 2922 | 32.721 | 35.209 | 21.442 | 1.00 55.46 |
| ATOM | 19589 | CG2 | THR | 2922 | 31.524 | 33.127 | 21.287 | 1.00 53.60 |
| | | | | | | | 22.476 | 1.00 56.52 |
| ATOM | 19590 | С | THR | 2922 | 30.394 | 36.593 | | 1.00 57.67 |
| ATOM | 19591 | 0 | THR | 2922 | 30.209 | 37.673 | 21.915 | |
| MOTA | 19592 | N | GLY | 2923 | 30.672 | 36.483 | 23.772 | 1.00 58.60 |
| ATOM | 19593 | CA | GLY | 2923 | 30.768 | 37.657 | 24.622 | 1.00 61.66 |
| MOTA | 19594 | C | GLY | 2923 | 31.545 | 38.803 | 24.004 | 1.00 63.68 |
| ATOM | 19595 | 0 | GLY | 2923 | 30.961 | 39.699 | 23.394 | 1.00 64.36 |
| MOTA | 19596 | N | GLY | 2924 | 32.864 | 38.779 | 24.162 | 1.00 64.67 |
| MOTA | 19597 | CA | GLY | 2924 | 33.688 | 39.835 | 23.607 | 1.00 66.50 |
| ATOM | 19598 | С | GLY | 2924 | 35.161 | 39.619 | 23.880 | 1.00 67.68 |
| ATOM | 19599 | 0 | GLY | 2924 | 36.015 | 39.989 | 23.072 | 1.00 68.28 |
| ATOM | 19600 | N | HIS | 2925 | 35.461 | 39.018 | 25.026 | 1.00 68.21 |
| ATOM | 19601 | CA | HIS | 2925 | 36.839 | 38.748 | 25.410 | 1.00 68.98 |
| ATOM | 19602 | CB | HIS | 2925 | 36.922 | 38.531 | 26.924 | 1.00 70.40 |
| ATOM | 19603 | CG | HIS | 2925 | 36.513 | 39.726 | 27.730 | 1.00 71.99 |
| | | | | | | 39.900 | 28.620 | 1.00 72.41 |
| ATOM | 19604 | CD2 | | 2925 | 35.508 | | | 1.00 72.41 |
| ATOM | 19605 | ND1 | | 2925 | 37.178 | 40.932 | 27.662 | |
| MOTA | 19606 | CE1 | | 2925 | 36.601 | 41.797 | 28.477 | 1.00 72.46 |
| ATOM | 19607 | | HIS. | 2925 | 35.585 | 41.197 | 29.070 | 1.00 72.60 |
| MOTA | 19608 | C | HIS | 2925 | 37.384 | 37.524 | 24.674 | 1.00 68.50 |
| ATOM | 19609 | 0 | HIS | 2925 | 37.745 | 36.524 | 25.294 | 1.00 68.44 |
| ATOM | 19610 | N | ILE | 2926 | 37.442 | 37.613 | 23.348 | 1.00 67.83 |
| ATOM | 19611 | CA | ILE | 2926 | 37.940 | 36.516 | 22.524 | 1.00 67.07 |
| ATOM | 19612 | CB | ILE | 2926 | 37.816 | 36.838 | 21.019 | 1.00 67.36 |
| ATOM | 19613 | CG2 | ILE | 2926 | 36.353 | 37.011 | 20.641 | 1.00 67.76 |
| MOTA | 19614 | CG1 | ILE | 2926 | 38.613 | 38.102 | 20.691 | 1.00 67.33 |
| ATOM | 19615 | CD1 | ILE | 2926 | 38.682 | 38.416 | 19.212 | 1.00 67.17 |
| ATOM | 19616 | С | ILE | 2926 | 39.406 | 36.224 | 22.827 | 1.00 66.38 |
| ATOM | 19617 | ō | ILE | 2926 | 40.136 | 37.094 | 23.300 | 1.00 66.76 |
| ATOM | 19618 | N | PRO | 2927 | 39.856 | 34.987 | 22.557 | 1.00 65.66 |
| ATOM | 19619 | CD | PRO | 2927 | 39.075 | 33.857 | 22.023 | 1.00 65.23 |
| ATOM | 19620 | CA | PRO | 2927 | 41.244 | 34.585 | 22.804 | 1.00 64.79 |
| | 19621 | CB | PRO | 2927 | 41.198 | 33.073 | 22.613 | 1.00 65.30 |
| ATOM | | | | | | | | |
| MOTA | 19622 | CG | PRO | 2927 | 40.158 | 32.914 | 21.553 | 1.00 65.30 |
| ATOM | 19623 | C | PRO | 2927 | 42.229 | 35.261 | 21.854 | 1.00 64.22 |
| ATOM | 19624 | 0 | PRO | 2927 | 41.838 | 35.812 | 20.824 | 1.00 63.39 |
| MOTA | 19625 | N | LYS | 2928 | 43.509 | 35.210 | 22.206 | 1.00 63.55 |
| MOTA | 19626 | CA | LYS | 2928 | 44.552 | 35.820 | 21.392 | 1.00 63.10 |
| MOTA | 19627 | CB | LYS | 2928 | 45.862 | 35.910 | 22.182 | 1.00 63.96 |
| MOTA | 19628 | CG | LYS | 2928 | 45.893 | 36.997 | 23.252 | 1.00 64.57 |
| MOTA | 19629 | CD | LYS | 2928 | 44.948 | 36.705 | 24.408 | 1.00 65.11 |
| ATOM | 19630 | CE | LYS | 2928 | 45.029 | 37.801 | 25.466 | 1.00 65.21 |
| ATOM | 19631 | NZ | LYS | 2928 | 44.169 | 37.518 | 26.651 | 1.00 64.88 |
| ATOM | 19632 | С | LYS | 2928 | 44.803 | 35.067 | 20.091 | 1.00 62.38 |
| ATOM | 19633 | 0 | LYS | 2928 | 45.363 | 35.622 | 19.145 | 1.00 62.12 |
| ATOM | 19634 | N | PHE | 2929 | 44.387 | 33.806 | 20.043 | 1.00 61.22 |
| ATOM | | CA | PHE | 2929 | 44.586 | 32.993 | 18.850 | 1.00 59.91 |
| ATOM | 19636 | СВ | PHE | 2929 | 44.905 | 31.550 | 19.248 | 1.00 59.84 |
| ATOM | 19637 | CG | PHE | 2929 | 43.882 | 30.926 | 20.154 | 1.00 60.10 |
| | 19638 | CD1 | | 2929 | 42.659 | 30.490 | 19.655 | 1.00 60.07 |
| MOTA | | | | | | 30.772 | | 1.00 60.07 |
| MOTA | 19639 | CD2 | | 2929 | 44.144 | | 21.511 | 1.00 59.46 |
| ATOM | 19640 | CE1 | | 2929 | 41.711 | 29.907 | 20.494 | |
| ATOM | 19641 | CE2 | | 2929 | 43.202 | 30.191 | 22.358 | 1.00 60.29 |
| MOTA | 19642 | CZ | PHE | 2929 | 41.983 | 29.758 | 21.848 | 1.00 59.76 |
| MOTA | 19643 | C | PHE | .2929 | 43.393 | 33.028 | 17.904 | 1.00 59.23 |
| MOTA | 19644 | 0 | PHE | 2929 | 43.370 | 32.321 | 16.897 | 1.00 59.32 |
| MOTA | 19645 | N | ALA | 2930 | 42.409 | 33.863 | | 1.00 57.98 |
| MOTA | 19646 | CA | ALA | 2930 | 41.212 | 33.995 | 17.404 | 1.00 56.99 |
| MOTA | 19647 | CB | ALA | 2930 | 39.967 | 33.889 | 18.273 | 1.00 56.84 |
| MOTA | 19648 | С | ALA | 2930 | 41.217 | 35.324 | 16.662 | 1.00 56.37 |
| ATOM | 19649 | 0 | ALA | 2930 | 42.091 | 36.161 | 16.876 | 1.00 56.26 |
| ATOM | 19650 | N | LYS | 2931 | 40.236 | 35.517 | 15.788 | 1.00 56.19 |
| MOTA | 19651 | CA | LYS | 2931 | 40.140 | 36.753 | 15.022 | 1.00 56.47 |
| ATOM | 19652 | CB | LYS | 2931 | 41.140 | 36.734 | 13.862 | 1.00 56.43 |
| ATOM | 19653 | CG | LYS | 2931 | 41.165 | 38.013 | 13.037 | 1.00 56.84 |
| ATOM | 19654 | CD | LYS | 2931 | 42.212 | 37.935 | 11.939 | 1.00 57.32 |
| ATOM | 19655 | CE | LYS | 2931 | 42.283 | 39.226 | 11.137 | 1.00 57.79 |
| | | | | | 42.263 | 39.151 | 10.053 | 1.00 57.79 |
| ATOM | 19656 | NZ | LYS | 2931 | | | | |
| ATOM | 19657 | C | LYS | 2931 | 38.730 | 36.963 | 14.481 | 1.00 56.42 |
| ATOM | 19658 | 0 | LYS | 2931 | 38.137 | 36.059 | 13.892 | 1.00 56.44 |
| ATOM | 19659 | N | ASN | 2932 | 38.202 | 38.165 | 14.687 | 1.00 56.03 |
| ATOM | 19660 | CA | ASN | 2932 | 36.867 | 38.510 | 14.220 | 1.00 55.89 |
| MOTA | 19661 | СВ | ASN | 2932 | 36.274 | 39.617 | 15.095 | 1.00 55.63 |
| ATOM | 19662 | CG | ASN | 2932 | 34.795 | 39.827 | 14.847 | 1.00 55.62 |
| MOTA | 19663 | OD1 | ASN | 2932 | 34.324 | 39.747 | 13.711 | 1.00 55.34 |
| | | | | | | | | |

| MOTA | 19664 | MD2 | ASN | 2932 | 34.053 | 40.111 | 15.911 | 1.00 55.48 |
|--------|-------|-----|-----|------|--------|----------|--------|------------|
| | | | | 2932 | 36.946 | 38.999 | 12.777 | 1.00 56.13 |
| ATOM | 19665 | C | ASN | | | | 12.527 | 1.00 56.78 |
| ATOM | 19666 | 0 | ASN | 2932 | 37.269 | 40.160 | | |
| MOTA | 19667 | N | PHE | 2933 | 36.656 | 38.115 | 11.829 | 1.00 56.14 |
| MOTA | 19668 | CA | PHE | 2933 | 36.697 | 38.482 | 10.422 | 1.00 57.27 |
| MOTA | 19669 | CB | PHE | 2933 | 36.817 | 37.234 | 9.543 | 1.00 57.12 |
| MOTA | 19670 | CG | PHE | 2933 | 38.141 | 36.540 | 9.658 | 1.00 57.30 |
| MOTA | 19671 | CD1 | PHE | 2933 | 38.472 | 35.829 | 10.807 | 1.00 56.85 |
| ATOM | 19672 | CD2 | PHE | 2933 | 39.073 | 36.621 | 8.627 | 1.00 57.13 |
| ATOM | 19673 | CE1 | PHE | 2933 | 39.713 | 35.209 | 10.927 | 1.00 57.60 |
| ATOM | 19674 | CE2 | | 2933 | 40.315 | 36.006 | 8.737 | 1.00 57.30 |
| | 19675 | CZ | PHE | 2933 | 40.637 | 35.299 | 9.889 | 1.00 57.81 |
| ATOM | | | | | 35.471 | | 10.009 | 1.00 58.04 |
| MOTA | 19676 | С | PHE | 2933 | | 39.284 | | |
| MOTA | 19677 | 0 | PHE | 2933 | 35.464 | 39.925 | 8.957 | 1.00 58.08 |
| MOTA | 19678 | N | LEU | 2934 | 34.432 | 39.242 | 10.837 | 1.00 59.10 |
| MOTA | 19679 | CA | LEU | 2934 | 33.205 | 39.980 | 10.556 | 1.00 59.92 |
| MOTA | 19680 | CB | LEU | 2934 | 32.050 | 39.449 | 11.409 | 1.00 58.78 |
| MOTA | 19681 | CG | LEU | 2934 | 30.721 | 40.200 | 11.278 | 1.00 58.03 |
| ATOM | 19682 | CD1 | LEU | 2934 | 30.222 | 40.120 | 9.844 | 1.00 57.10 |
| MOTA | 19683 | CD2 | LEU | 2934 | 29.698 | 39.610 | 12.232 | 1.00 57.76 |
| MOTA | 19684 | С | LEU | 2934 | 33.426 | 41.454 | 10.864 | 1.00 61.04 |
| MOTA | 19685 | 0 | LEU | 2934 | 32.864 | 42.326 | 10.204 | 1.00 61.19 |
| ATOM | 19686 | N | ALA | 2935 | 34.247 | 41.721 | 11.874 | 1.00 62.38 |
| ATOM | 19687 | CA | ALA | 2935 | 34.552 | 43.086 | 12.274 | 1.00 64.22 |
| | | CB | ALA | 2935 | 35.328 | 43.085 | 13.583 | 1.00 63.92 |
| MOTA | 19688 | | | | | | | |
| MOTA | 19689 | C | ALA | 2935 | 35.362 | 43.775 | 11.182 | 1.00 65.41 |
| MOTA | 19690 | 0 | ALA | 2935 | 35.204 | 44.972 | 10.935 | 1.00 65.96 |
| MOTA | 19691 | N | GLU | 2936 | 36.229 | 43.005 | 10.529 | 1.00 66.66 |
| ATOM ' | 19692 | CA | GLU | 2936 | 37.070 | 43.523 | 9.454 | 1.00 67.61 |
| ATOM | 19693 | CB | GLU | 2936 | 38.167 | 42.511 | 9.105 | 1.00 68.36 |
| ATOM | 19694 | CG | GLU | 2936 | 38.961 | 41.982 | 10.294 | 1.00 69.12 |
| ATOM | 19695 | CD | GLU | 2936 | 39.699 | 43.070 | 11.051 | 1.00 69.89 |
| ATOM | 19696 | OE1 | GLU | 2936 | 39.034 | 43.903 | 11.703 | 1.00 70.02 |
| ATOM | 19697 | OE2 | GLU | 2936 | 40.948 | 43.094 | 10.989 | 1.00 70.26 |
| ATOM | 19698 | C | GLU | 2936 | 36.216 | 43.788 | 8.217 | 1.00 67.80 |
| ATOM | 19699 | 0 | GLU | 2936 | 36.719 | 44.238 | 7.187 | 1.00 67.71 |
| | | | | | | | | |
| ATOM | 19700 | N | THR | 2937 | 34.923 | 43.497 | 8.328 | 1.00 67.74 |
| ATOM | 19701 | CA | THR | 2937 | 33.988 | 43.696 | 7.228 | 1.00 67.18 |
| MOTA | 19702 | CB | THR | 2937 | 33.961 | 42.455 | 6.306 | 1.00 67.51 |
| ATOM | 19703 | OG1 | THR | 2937 | 33.149 | 42.726 | 5.157 | 1.00 67.78 |
| MOTA | 19704 | CG2 | THR | 2937 | 33.399 | 41.249 | 7.048 | 1.00 67.76 |
| ATOM | 19705 | С | THR | 2937 | 32.577 | 43.974 | 7.757 | 1.00 66.84 |
| ATOM | 19706 | 0 | THR | 2937 | 32.410 | 44.481 | 8.869 | 1.00 66.83 |
| MOTA | 19707 | N | GLY | 2938 | 31.565 | 43.650 | 6.958 | 1.00 66.24 |
| ATOM | 19708 | CA | GLY | 2938 | 30.192 | 43.873 | 7.374 | 1.00 65.54 |
| ATOM | 19709 | C | GLY | 2938 | 29.275 | 42.763 | 6.899 | 1.00 64.98 |
| ATOM | 19710 | 0 | GLY | 2938 | 28.054 | 42.842 | 7.043 | 1.00 64.61 |
| | | | | | | | | 1.00 64.32 |
| ATOM | 19711 | N | ASP | 2939 | 29.874 | 41.721 | 6.331 | |
| MOTA | 19712 | CA | ASP | 2939 | 29.123 | 40.582 | 5.822 | 1.00 63.45 |
| MOTA | 19713 | CB | ASP | 2939 | 29.128 | 40.595 | 4.291 | 1.00 64.45 |
| ATOM | 19714 | CG | ASP | 2939 | 28.216 | 39.544 | 3.698 | 1.00 65.72 |
| ATOM | 19715 | OD1 | ASP | 2939 | 28.488 | 38.340 | 3.889 | 1.00 66.50 |
| ATOM | 19716 | OD2 | ASP | 2939 | 27.222 | 39.924 | 3.042 | 1.00 66.35 |
| ATOM | 19717 | С | ASP | 2939 | 29.725 | 39.277 | 6.336 | 1.00 62.43 |
| ATOM | 19718 | 0 | ASP | 2939 | 30.928 | 39.044 | 6.209 | 1.00 61.79 |
| ATOM | 19719 | N | ILE | 2940 | 28.878 | 38.433 | 6.920 | 1.00 61.10 |
| MOTA | 19720 | CA | ILE | 2940 | 29.310 | 37.148 | 7.463 | 1.00 59.37 |
| ATOM | 19721 | CB | ILE | 2940 | 28.105 | 36.342 | 8.007 | 1.00 59.30 |
| ATOM | 19722 | CG2 | ILE | 2940 | 28.577 | 34.996 | 8.539 | 1.00 59.02 |
| ATOM | 19723 | CG1 | ILE | 2940 | 27.404 | 37.136 | 9.113 | 1.00 59.59 |
| | | | | | | | 9.656 | 1.00 59.03 |
| ATOM | 19724 | CD1 | | 2940 | 26.152 | 36.472 | | |
| ATOM | 19725 | C | ILE | 2940 | 30.026 | 36.308 | 6.408 | 1.00 58.22 |
| ATOM | 19726 | 0 | ILE | 2940 | 31.116 | 35.792 | 6.652 | 1.00 57.54 |
| MOTA | 19727 | N | ARG | 2941 | 29.407 | 36.171 | 5.240 | 1.00 57.25 |
| MOTA | 19728 | CA | ARG | 2941 | 29.991 | 35.395 | 4.154 | 1.00 56.77 |
| MOTA | 19729 | CB | ARG | 2941 | 29.033 | 35.348 | 2.963 | 1.00 55.80 |
| ATOM | 19730 | CG | ARG | 2941 | 27.778 | · 34.525 | 3.206 | 1.00 53.72 |
| MOTA | 19731 | CD | ARG | 2941 | 26.838 | 34.590 | 2.013 | 1.00 52.37 |
| ATOM | 19732 | NE | ARG | 2941 | 25.691 | 33.698 | 2.165 | 1.00 51.33 |
| ATOM | 19733 | CZ | ARG | 2941 | 24.805 | 33.775 | 3.153 | 1.00 50.67 |
| ATOM | 19734 | | ARG | 2941 | 24.927 | 34.706 | 4.089 | 1.00 50.47 |
| ATOM | | NH2 | | | 23.793 | 32.919 | 3.204 | 1.00 50.47 |
| | 19735 | | | 2941 | | | 3.721 | |
| ATOM | 19736 | C | ARG | 2941 | 31.328 | 35.986 | | 1.00 57.51 |
| ATOM | 19737 | 0 | ARG | 2941 | 32.278 | 35.254 | 3.441 | 1.00 58.07 |
| ATOM | 19738 | N | ALA | 2942 | 31.394 | 37.313 | 3.666 | 1.00 57.53 |
| MOTA | 19739 | CA | ALA | 2942 | 32.618 | 38.001 | 3.275 | 1.00 57.14 |
| ATOM | 19740 | CB | ALA | 2942 | 32.384 | 39.506 | 3.243 | 1.00 57.24 |

| MOTA | 19741 | C | ALA | 2942 | 33.729 | 37.663 | 4.262 | 1.00 56.97 |
|------|-------|-----|-----|------|--------|--------|--------|------------|
| ATOM | 19742 | 0 | ALA | 2942 | 34.882 | 37.475 | 3.874 | 1.00 57.28 |
| ATOM | 19743 | N | ALA | 2943 | 33.372 | 37.584 | 5.540 | 1 00 56.48 |
| ATOM | 19744 | CA | ALA | 2943 | 34.338 | 37.263 | 6.583 | 1.00 56.25 |
| | 19745 | СВ | ALA | 2943 | 33.679 | 37.359 | 7.950 | 1.00 56.65 |
| MOTA | | | | | | | 6.368 | |
| MOTA | 19746 | C | ALA | 2943 | 34.896 | 35.861 | | 1.00 56.16 |
| ATOM | 19747 | 0 | ALA | 2943 | 36.044 | 35.583 | 6.712 | 1.00 56.09 |
| MOTA | 19748 | N | VAL | 2944 | 34.077 | 34.984 | 5.792 | 1.00 56.16 |
| ATOM | 19749 | CA | VAL | 2944 | 34.485 | 33.609 | 5.526 | 1.00 55.63 |
| ATOM | 19750 | CB | VAL | 2944 | 33.279 | 32.735 | 5.106 | 1.00 56.09 |
| ATOM | 19751 | | VAL | 2944 | 33.745 | 31.318 | 4.801 | 1.00 55.49 |
| ATOM | 19752 | CG2 | VAL | 2944 | 32.234 | 32.722 | 6.213 | 1.00 55.66 |
| | | C | | 2944 | 35.532 | 33.557 | 4.420 | 1.00 55.75 |
| ATOM | 19753 | | VAL | | | | | |
| MOTA | 19754 | 0 | VAL | 2944 | 36.568 | 32.909 | 4.569 | 1.00 55.47 |
| MOTA | 19755 | N | ARG | 2945 | 35.257 | 34.238 | 3.311 | 1.00 55.89 |
| MOTA | 19756 | CA | ARG | 2945 | 36.188 | 34.264 | 2.189 | 1.00 55.76 |
| MOTA | 19757 | CB | ARG | 2945 | 35.622 | 35.094 | 1.034 | 1.00 55.60 |
| ATOM | 19758 | CG | ARG | 2945 | 34.413 | 34.471 | 0.356 | 1.00 56.71 |
| MOTA | 19759 | CD | ARG | 2945 | 34.101 | 35.175 | -0.956 | 1.00 57.24 |
| ATOM | 19760 | NE | ARG | 2945 | 33.775 | 36.585 | -0.762 | 1.00 57.48 |
| ATOM | 19761 | CZ | ARG | 2945 | 32.653 | 37.024 | -0.199 | 1.00 57.88 |
| | | | | | | | 0.228 | |
| ATOM | 19762 | | ARG | 2945 | 31.740 | 36.163 | | |
| MOTA | 19763 | NH2 | | 2945 | 32.445 | 38.327 | -0.061 | 1.00 57.70 |
| MOTA | 19764 | С | ARG | 2945 | 37.532 | 34.836 | 2.617 | 1.00 55.48 |
| MOTA | 19765 | 0 | ARG | 2945 | 38.585 | 34.335 | 2.216 | 1.00 55.77 |
| ATOM | 19766 | N | GLN | 2946 | 37.491 | 35.886 | 3.431 | 1.00 54.96 |
| ATOM | 19767 | CA | GLN | 2946 | 38.710 | 36.520 | 3.918 | 1.00 54.60 |
| ATOM | 19768 | CB | GLN | 2946 | 38.368 | 37.747 | 4.769 | 1.00 55.75 |
| ATOM | 19769 | CG | GLN | 2946 | 39.574 | 38.580 | 5.179 | 1.00 57.10 |
| | | | | 2946 | 39.215 | 39.681 | 6.161 | 1.00 58.43 |
| MOTA | 19770 | CD | GLN | | | | | |
| ATOM | 19771 | OE1 | | 2946 | 38.307 | 40.478 | 5.917 | 1.00 59.03 |
| MOTA | 19772 | NE2 | GLN | 2946 | 39.932 | 39.733 | 7.279 | 1.00 58.79 |
| MOTA | 19773 | С | GLN | 2946 | 39.482 | 35.509 | 4.757 | 1.00 53.60 |
| ATOM | 19774 | 0 | GLN | 2946 | 40.707 | 35.416 | 4.670 | 1.00 53.90 |
| ATOM | 19775 | N | TYR | 2947 | 38.752 | 34.754 | 5.571 | 1.00 52.23 |
| ATOM | 19776 | CA | TYR | 2947 | 39.350 | 33.736 | 6.426 | 1.00 50.90 |
| ATOM | 19777 | CB | TYR | 2947 | 38.267 | 33.086 | 7.291 | 1.00 49.81 |
| | | | | 2947 | 38.721 | 31.849 | 8.030 | 1.00 48.86 |
| MOTA | 19778 | CG | TYR | | | | | |
| ATOM | 19779 | CD1 | TYR | 2947 | 39.824 | 31.887 | 8.882 | 1.00 48.05 |
| MOTA | 19780 | CE1 | TYR | 2947 | 40.240 | 30.751 | 9.570 | 1.00 48.01 |
| ATOM | 19781 | CD2 | TYR | 2947 | 38.042 | 30.639 | 7.884 | 1.00 48.25 |
| MOTA | 19782 | CE2 | TYR | 2947 | 38.449 | 29.497 | 8.567 | 1.00 47.92 |
| ATOM | 19783 | CZ | TYR | 2947 | 39.548 | 29.559 | 9.408 | 1.00 48.00 |
| ATOM | 19784 | ОН | TYR | 2947 | 39.957 | 28.434 | 10.087 | 1.00 46.78 |
| ATOM | 19785 | C | TYR | 2947 | 40.045 | 32.679 | 5.574 | 1.00 50.61 |
| ATOM | 19786 | Õ | TYR | 2947 | 41.195 | 32.315 | 5.828 | 1.00 50.43 |
| ATOM | 19787 | N | | 2948 | 39.333 | 32.194 | 4.562 | 1.00 50.53 |
| | | | MET | | | | | |
| MOTA | 19788 | CA | MET | 2948 | 39.856 | 31.183 | 3.652 | 1.00 50.34 |
| MOTA | 19789 | CB | MET | 2948 | 38.785 | 30.803 | 2.627 | 1.00 50.02 |
| MOTA | 19790 | CG | MET | 2948 | 37.518 | 30.204 | 3.220 | 1.00 47.76 |
| MOTA | 19791 | SD | MET | 2948 | 36.190 | 30.122 | 1.998 | 1.00 48.64 |
| MOTA | 19792 | CE | MET | 2948 | 36.932 | 29.063 | 0.769 | 1.00 48.77 |
| MOTA | 19793 | С | MET | 2948 | 41.094 | 31.701 | 2.921 | 1.00 51.03 |
| MOTA | 19794 | 0 | MET | 2948 | 42.109 | 31.008 | 2.827 | 1.00 51.21 |
| ATOM | 19795 | N | ALA | 2949 | 41.001 | 32.923 | 2.407 | 1.00 50.88 |
| ATOM | 19796 | CA | ALA | 2949 | 42.103 | 33.533 | 1.674 | 1.00 51.33 |
| ATOM | 19797 | CB | ALA | 2949 | 41.640 | 34.835 | 1.033 | 1.00 51.05 |
| | | | | | | | | |
| ATOM | 19798 | C | ALA | 2949 | 43.328 | 33.789 | 2.547 | |
| MOTA | 19799 | 0 | ALA | 2949 | 44.457 | 33.528 | 2.128 | 1.00 52.35 |
| MOTA | 19800 | N | GLU | 2950 | 43.112 | 34.296 | 3.758 | 1.00 52.03 |
| MOTA | 19801 | CA | GLU | 2950 | 44.222 | 34.583 | 4.662 | 1.00 52.73 |
| MOTA | 19802 | CB | GLU | 2950 | 43.735 | 35.373 | 5.880 | 1.00 52.54 |
| ATOM | 19803 | CG | GLU | 2950 | 43.593 | 36.864 | 5.622 | 1.00 53.18 |
| ATOM | 19804 | CD | GLU | 2950 | 43.213 | 37.643 | 6.867 | 1.00 53.56 |
| ATOM | 19805 | | GLU | 2950 | 43.847 | 37.429 | 7.923 | 1.00 53.35 |
| ATOM | 19806 | OE2 | | 2950 | 42.287 | 38.478 | 6.787 | 1.00 54.33 |
| | | | | | | | | 1.00 54.33 |
| ATOM | 19807 | C | GLU | 2950 | 44.971 | 33.340 | 5.128 | |
| MOTA | 19808 | 0 | GLU | 2950 | 46.168 | 33.404 | 5.413 | 1.00 53.12 |
| MOTA | 19809 | N | VAL | 2951 | 44.272 | 32.213 | 5.210 | 1.00 53.26 |
| MOTA | 19810 | CA | VAL | 2951 | 44.903 | 30.971 | 5.641 | 1.00 53.29 |
| ATOM | 19811 | CB | VAL | 2951 | 43.849 | 29.891 | 5.970 | 1.00 53.31 |
| ATOM | 19812 | CG1 | VAL | 2951 | 44.533 | 28.561 | 6.259 | 1.00 53.04 |
| MOTA | 19813 | CG2 | | 2951 | 43.025 | 30.327 | 7.174 | 1.00 52.46 |
| ATOM | 19814 | С | VAL | 2951 | 45.849 | 30.442 | 4.568 | 1.00 53.26 |
| ATOM | 19815 | ŏ | VAL | 2951 | 47.012 | 30.145 | 4.847 | 1.00 53.25 |
| ATOM | 19816 | N | GLU | 2952 | 45.348 | 30.328 | 3.342 | 1.00 53.25 |
| | | | | | | 29.835 | 2.232 | |
| MOTA | 19817 | CA | GLU | 2952 | 46.157 | 47.033 | 4.434 | 1.00 54.22 |
| | | | | | | | | |

| MOTA | 19818 | CB | GLU | 2952 | 45.328 | 29.793 | 0.947 | 1.00 54.72 |
|------|-------|-----|-----|------|--------|--------|--------|------------|
| ATOM | 19819 | CG | GLU | 2952 | 46.082 | 29.252 | -0.261 | 1.00 55.51 |
| ATOM | 19820 | CD | GLU | 2952 | 45.257 | 29.300 | -1.532 | 1.00 56.73 |
| | | | | | 45.774 | 28.890 | -2.594 | 1.00 57.69 |
| MOTA | 19821 | OE1 | | 2952 | | | | |
| MOTA | 19822 | OE2 | GLU | 2952 | 44.092 | 29.750 | -1.473 | 1.00 56.56 |
| MOTA | 19823 | C | GLU | 2952 | 47.370 | 30.730 | 2.023 | 1.00 54.22 |
| MOTA | 19824 | 0 | GLU | 2952 | 48.430 | 30.266 | 1.608 | 1.00 54.53 |
| ATOM | 19825 | N | SER | 2953 | 47.202 | 32.015 | 2.318 | 1.00 54.17 |
| ATOM | 19826 | CA | SER | 2953 | 48.272 | 32.993 | 2.162 | 1.00 54.43 |
| ATOM | 19827 | СВ | SER | 2953 | 47.690 | 34.407 | 2.129 | 1.00 54.29 |
| ATOM | 19828 | OG | SER | 2953 | 46.736 | 34.542 | 1.092 | 1.00 56.12 |
| | | | | | 49.279 | 32.892 | 3.297 | 1.00 54.04 |
| MOTA | 19829 | C | SER | 2953 | | | | |
| ATOM | 19830 | 0 | SER | 2953 | 50.487 | 32.943 | 3.074 | 1.00 54.27 |
| MOTA | 19831 | N | GLY | 2954 | 48.771 | 32.750 | 4.516 | 1.00 53.77 |
| ATOM | 19832 | CA | GLY | 2954 | 49.642 | 32.657 | 5.672 | 1.00 53.06 |
| ATOM | 19833 | С | GLY | 2954 | 49.442 | 33.832 | 6.609 | 1.00 52.88 |
| ATOM | 19834 | 0 | GLY | 2954 | 49.975 | 33.854 | 7.719 | 1.00 51.86 |
| ATOM | 19835 | N | VAL | 2955 | 48.670 | 34.815 | 6.156 | 1.00 52.98 |
| ATOM | 19836 | CA | VAL | 2955 | 48.388 | 36.003 | 6.953 | 1.00 53.65 |
| | | | | | | | | |
| ATOM | 19837 | CB | VAL | 2955 | 47.426 | 36.952 | 6.214 | 1.00 54.01 |
| MOTA | 19838 | CG1 | | 2955 | 47.201 | 38.208 | 7.039 | 1.00 53.59 |
| ATOM | 19839 | CG2 | VAL | 2955 | 47.990 | 37.300 | 4.846 | 1.00 54.14 |
| ATOM | 19840 | С | VAL | 2955 | 47.756 | 35.606 | 8.281 | 1.00 54.39 |
| ATOM | 19841 | 0 | VAL | 2955 | 48.003 | 36.236 | 9.309 | 1.00 53.92 |
| ATOM | 19842 | N | TYR | 2956 | 46.934 | 34.560 | 8.249 | 1.00 54.97 |
| ATOM | 19843 | CA | TYR | 2956 | 46.271 | 34.070 | 9.451 | 1.00 55.91 |
| ATOM | 19844 | CB | TYR | 2956 | 44.756 | 34.258 | 9.346 | 1.00 56.40 |
| | | | | | 44.014 | 33.837 | 10.595 | 1.00 57.63 |
| ATOM | 19845 | CG | TYR | 2956 | • . | | | |
| MOTA | 19846 | CD1 | TYR | 2956 | 44.082 | 34.600 | 11.761 | 1.00 57.68 |
| MOTA | 19847 | CE1 | TYR | 2956 | 43.423 | 34.202 | 12.923 | 1.00 58.33 |
| MOTA | 19848 | CD2 | TYR | 2956 | 43.265 | 32.660 | 10.621 | 1.00 58.32 |
| ATOM | 19849 | CE2 | TYR | 2956 | 42.603 | 32.251 | 11.778 | 1.00 58.41 |
| MOTA | 19850 | CZ | TYR | 2956 | 42.686 | 33.027 | 12.924 | 1.00 58.65 |
| MOTA | 19851 | ОН | TYR | 2956 | 42.033 | 32.631 | 14.069 | 1.00 58.77 |
| ATOM | 19852 | C | TYR | 2956 | 46.577 | 32.591 | 9.675 | 1.00 56.09 |
| | | | | 2956 | | 31.779 | 8.754 | 1.00 56.17 |
| MOTA | 19853 | 0 | TYR | | 46.478 | | | |
| MOTA | 19854 | N | PRO | 2957 | 46.962 | 32.223 | 10.908 | 1.00 56.16 |
| MOTA | 19855 | CD | PRO | 2957 | 47.177 | 30.824 | 11.320 | 1.00 56.15 |
| MOTA | 19856 | CA | PRO | 2957 | 47.109 | 33.126 | 12.052 | 1.00 56.59 |
| MOTA | 19857 | CB | PRO | 2957 | 47.081 | 32.173 | 13.239 | 1.00 56.39 |
| MOTA | 19858 | CG | PRO | 2957 | 47.791 | 30.980 | 12.698 | 1.00 56.47 |
| MOTA | 19859 | C | PRO | 2957 | 48.405 | 33.928 | 11.984 | 1.00 57.30 |
| ATOM | 19860 | 0 | PRO | 2957 | 49.413 | 33.452 | 11.462 | 1.00 57.47 |
| ATOM | 19861 | N | GLY | 2958 | 48.370 | 35.148 | 12.512 | 1.00 58.29 |
| | 19862 | ĊÀ | GLY | 2958 | 49.551 | 35.991 | 12.504 | 1.00 59.19 |
| ATOM | | | | | | | | |
| MOTA | 19863 | С | GLY | 2958 | 50.469 | 35.674 | 13.668 | 1.00 59.90 |
| MOTA | 19864 | 0 | GLY | 2958 | 50.359 | 34.612 | 14.282 | 1.00 59.93 |
| MOTA | 19865 | N | GLU | 2959 | 51.376 | 36.595 | 13.975 | 1.00 60.38 |
| MOTA | 19866 | CA | GLU | 2959 | 52.312 | 36.400 | 15.076 | 1.00 60.87 |
| MOTA | 19867 | CB | GLU | 2959 | 53.457 | 37.413 | 14.988 | 1.00 61.40 |
| ATOM | 19868 | CG | GLU | 2959 | 54.521 | 37.227 | 16.060 | 1.00 61.82 |
| АТОМ | 19869 | CD | GLU | 2959 | 55.285 | 35.926 | 15.903 | 1.00 62.12 |
| ATOM | 19870 | | GLU | 2959 | 56.067 | 35.579 | 16.813 | 1.00 62.78 |
| ATOM | | | GLU | 2959 | 55.108 | 35.251 | 14.867 | 1.00 62.30 |
| | 19871 | | | 2959 | | | 16.419 | 1.00 60.84 |
| ATOM | 19872 | С | GLU | | 51.605 | 36.548 | | |
| ATOM | 19873 | 0 | GLU | 2959 | 51.933 | 35.855 | 17.384 | 1.00 60.59 |
| ATOM | 19874 | N | GLU | 2960 | 50.634 | 37.454 | 16.477 | 1.00 61.19 |
| MOTA | 19875 | CA | GLU | 2960 | 49.889 | 37.689 | 17.709 | 1.00 61.99 |
| MOTA | 19876 | CB | GLU | 2960 | 48.941 | 38.882 | 17.554 | 1.00 62.57 |
| MOTA | 19877 | CG | GLU | 2960 | 49.390 | 39.924 | 16.546 | 1.00 63.87 |
| MOTA | 19878 | CD | GLU | 2960 | 49.017 | 39.551 | 15.123 | 1.00 64.41 |
| ATOM | 19879 | OE1 | | 2960 | | 39.475 | 14.828 | 1.00 64.20 |
| ATOM | 19880 | OE2 | | 2960 | 49.933 | 39.330 | 14.301 | 1.00 64.88 |
| ATOM | 19881 | C | GLU | 2960 | 49.077 | 36.450 | 18.052 | 1.00 61.91 |
| ATOM | 19882 | | GLU | 2960 | 48.947 | 36.081 | 19.219 | 1.00 62.32 |
| | | 0 | | | | | | |
| MOTA | 19883 | N | HIS | 2961 | 48.534 | 35.813 | 17.020 | 1.00 61.34 |
| ATOM | 19884 | CA | HIS | 2961 | 47.723 | 34.615 | 17.196 | 1.00 60.73 |
| MOTA | 19885 | CB | HIS | 2961 | 46.855 | 34.386 | 15.957 | 1.00 59.89 |
| MOTA | 19886 | CG | HIS | 2961 | 46.116 | 35.607 | 15.504 | 1.00 58.97 |
| ATOM | 19887 | CD2 | HIS | 2961 | 46.080 | 36.231 | 14.302 | 1.00 58.22 |
| ATOM | 19888 | | HIS | 2961 | 45.285 | 36.326 | 16.334 | 1.00 58.84 |
| ATOM | 19889 | | HIS | 2961 | 44.768 | 37.341 | 15.665 | 1.00 58.19 |
| ATOM | 19890 | | HIS | 2961 | 45.233 | 37.306 | 14.430 | 1.00 57.99 |
| ATOM | 19891 | C | | 2961 | 48.599 | | 17.437 | 1.00 60.75 |
| | | | HIS | | | 33.391 | | |
| ATOM | 19892 | 0 | HIS | 2961 | 48.106 | 32.261 | 17.467 | 1.00 60.65 |
| ATOM | 19893 | N | SER | 2962 | 49.897 | 33.619 | 17.614 | 1.00 60.45 |
| ATOM | 19894 | CA | SER | 2962 | 50.839 | 32.529 | 17.844 | 1.00 60.48 |
| | | | | | | | | |

| ATOM | 19895 | CB | SER | 2962 | 52.007 | 32.630 | 16.862 | 1.00 60.35 |
|-------|-------|------|----------------------------------|------|---------|---------|---------|------------|
| ATOM | 19896 | OG | SER | 2962 | 51.552 | 32.553 | 15.522 | 1.00 59.02 |
| ATOM | 19897 | C | SER | 2962 | 51.370 | 32.518 | 19.273 | 1.00 60.73 |
| MOTA | 19898 | ŏ | SER | 2962 | 51.339 | 33.534 | 19.964 | 1.00 60.10 |
| ATOM | 19899 | N | PHE | 2963 | 51.851 | 31.356 | 19.708 | 1.00 61.57 |
| | | | | | | 31.194 | 21.053 | 1.00 62.25 |
| ATOM | 19900 | CA | PHE | 2963 | 52.394 | | | |
| ATOM | 19901 | CB | PHE | 2963 | 51.644 | 30.091 | 21.807 | 1.00 63.03 |
| MOTA | 19902 | CG | PHE | 2963 | 50.248 | 30.470 | 22.214 | 1.00 64.44 |
| MOTA | 19903 | CD1 | | 2963 | 49.278 | 30.750 | 21.256 | 1.00 64.83 |
| MOTA | 19904 | CD2 | PHE | 2963 | 49.903 | 30.552 | 23.560 | 1.00 64.71 |
| MOTA | 19905 | CE1 | PHE | 2963 | 47.983 | 31.107 | 21.632 | 1.00 64.99 |
| MOTA | 19906 | CE2 | PHE | 2963 | 48.614 | 30.906 | 23.948 | 1.00 65.11 |
| MOTA | 19907 | CZ | PHE | 2963 | 47.651 | 31.185 | 22.981 | 1.00 65.30 |
| ATOM | 19908 | С | PHE | 2963 | 53.880 | 30.853 | 21.006 | 1.00 62.31 |
| ATOM | 19909 | O | PHE | 2963 | 54.379 | 30.323 | 20.011 | 1.00 61.84 |
| ATOM | 19910 | N | HIS | 2964 | 54.577 | 31.156 | 22.096 | 1.00 62.35 |
| ATOM | 19911 | CA | HIS | 2964 | 56.007 | 30.897 | 22.201 | 1.00 62.42 |
| MOTA | 19912 | CB | HIS | 2964 | 56.795 | 32.135 | 21.772 | 1.00 62.17 |
| ATOM | 19913 | CG | HIS | 2964 | 56.654 | 32.468 | 20.318 | 1.00 62.21 |
| | 19914 | | HIS | 2964 | 56.082 | 33.526 | 19.696 | 1.00 62.06 |
| MOTA | | | HIS | 2964 | 57.137 | 31.652 | 19.319 | 1.00 62.06 |
| MOTA | 19915 | | | | | | | |
| MOTA | 19916 | | HIS | 2964 | 56.870 | 32.193 | 18.143 | 1.00 62.55 |
| MOTA | 19917 | | HIS | 2964 | 56.230 | 33.330 | 18.344 | 1.00 62.23 |
| MOTA | 19918 | С | HIS | 2964 | 56.382 | 30.514 | 23.628 | 1.00 62.87 |
| MOTA | 19919 | 0 | HIS | 2964 | 57.101 | 29.507 | 23.800 | 1.00 63.17 |
| MOTA | 19920 | ОХТ | HIS | 2964 | 55.958 | 31.232 | 24.558 | 1.00 63.88 |
| MOTA | 19921 | C1 | KPL | 2965 | 38.359 | 24.260 | 19.395 | 1.00 44.32 |
| MOTA | 19922 | C2 | KPL | 2965 | 38.509 | 22.957 | 18.586 | 1.00 44.37 |
| ATOM | 19923 | C3 | KPL | 2965 | 38.070 | 23.219 | 17.138 | 1.00 44.11 |
| ATOM | 19924 | C4 | KPL | 2965 | 39.994 | 22.528 | 18.576 | 1.00 44.41 |
| MOTA | 19925 | 01 | KPL | 2965 | 40.466 | 22.273 | 19.906 | 1.00 46.59 |
| ATOM | 19926 | C5 | KPL | 2965 | 37.616 | 21.846 | 19.201 | 1.00 44.46 |
| ATOM | 19927 | 02 | KPL | 2965 | 38.120 | 20.811 | 19.596 | 1.00 45.29 |
| ATOM | 19928 | C6 | KPL | 2965 | 36.112 | 22.005 | 19.331 | 1.00 44.39 |
| | 19929 | 03 | KPL | 2965 | 35.550 | 23.016 | 18.951 | 1.00 44.59 |
| MOTA | | | | | 35.382 | | 19.874 | 1.00 43.64 |
| ATOM | 19930 | 04 | KPL | 2965 | | 21.012 | | |
| ATOM | 19931 | | | 3001 | 3.994 | 24.216 | 47.085 | 1.00 41.37 |
| MOTA | 19932 | | | 3002 | 6.567 | 28.508 | 15.105 | 1.00 41.66 |
| MOTA | 19933 | | | 3003 | -3.352 | 1.040 | 0.322 | 1.00 26.64 |
| ATOM. | 19934 | | | 3004 | -12.375 | -19.811 | 23.437 | 1.00 24.57 |
| MOTA | 19935 | MG+2 | MG2 | 3005 | -7.605 | -5.894 | 52.220 | 1.00 34.50 |
| MOTA | 19936 | MG+2 | MG2 | 3006 | 27.460 | -4.705 | 0.894 | 1.00 30.26 |
| ATOM | 19937 | MG+2 | MG2 | 3007 | 17.331 | -30.253 | 18.884 | 1.00 32.29 |
| MOTA | 19938 | MG+2 | MG2 | 3008 | 19.663 | -21.554 | 49.976 | 1.00 25.48 |
| MOTA | 19939 | MG+2 | MG2 | 3009 | 31.302 | 8.730 | 51.343 | 1.00 41.34 |
| ATOM | 19940 | MG+2 | MG2 | 3010 | 36.277 | 19.579 | 21.091 | 1.00 52.60 |
| ATOM | 19941 | OH2 | WAT | 3011 | 31.424 | -16.107 | 39.470 | 1.00 10.76 |
| ATOM | 19942 | | WAT | 3012 | 12.698 | -18.611 | 32.844 | 1.00 10.49 |
| ATOM | 19943 | | TAW | 3013 | -8.246 | 1.949 | 11.544 | 1.00 13.19 |
| ATOM | 19944 | | WAT | 3014 | 27.207 | -31.545 | 22.513 | 1.00 13.62 |
| ATOM | 19945 | | WAT | 3015 | 25.517 | -21.182 | 20.257 | 1.00 10.14 |
| ATOM | 19946 | | WAT | 3016 | | 17.525 | | 1.00 13.74 |
| | | | | | -2.159 | -6.488 | 21.338 | 1.00 15.74 |
| ATOM | 19947 | | TAW | 3017 | | | | 1.00 15.76 |
| MOTA | 19948 | | TAW | 3018 | 0.835 | -9.327 | 15.447 | |
| ATOM | 19949 | | WAT | 3019 | | -32.000 | 22.104 | 1.00 11.84 |
| ATOM | 19950 | | WAT | 3020 | 37.123 | -1.512 | 39.521 | 1.00 16.58 |
| ATOM | 19951 | | TAW | 3021 | 17.933 | -46.120 | 14.538 | 1.00 11.66 |
| ATOM | 19952 | | TAW | 3022 | 10.775 | -17.843 | 17.172 | 1.00 15.20 |
| MOTA | 19953 | | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3023 | | -11.897 | 13.470 | 1.00 11.48 |
| ATOM | 19954 | | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3024 | -14.336 | | -15.394 | 1.00 13.53 |
| MOTA | 19955 | OH2 | TAW | 3025 | 12.577 | -9.564 | 9.580 | 1.00 14.31 |
| MOTA | 19956 | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3026 | -23.367 | 12.451 | 2.123 | 1.00 20.69 |
| MOTA | 19957 | OH2 | TAW | 3027 | 0.767 | -19.320 | 30.486 | 1.00 16.05 |
| ATOM | 19958 | | TAW | 3028 | -0.982 | -8.203 | 33.657 | 1.00 15.14 |
| ATOM | 19959 | | WAT | 3029 | 5.689 | 5.614 | 45.308 | 1.00 11.24 |
| ATOM | 19960 | | WAT | 3030 | 4.143 | 4.088 | 43.662 | 1.00 15.33 |
| ATOM | 19961 | OH2 | | 3031 | -16.843 | -2.595 | 47.938 | 1.00 11.00 |
| ATOM | 19962 | | WAT | 3032 | 12.241 | 13.450 | 38.158 | 1.00 23.70 |
| ATOM | 19963 | | WAT | 3032 | -5.960 | -12.449 | 28.625 | 1.00 14.48 |
| ATOM | 19964 | | | 3034 | | -12.732 | 16.031 | 1.00 14.45 |
| | | | WAT | | | | 37.635 | 1.00 14.41 |
| ATOM | 19965 | | TAW | 3035 | | -17.361 | | |
| MOTA | 19966 | | TAW | 3036 | 29.576 | -3.425 | 53.736 | 1.00 16.58 |
| MOTA | 19967 | | WAT | 3037 | | -14.473 | 37.183 | 1.00 18.91 |
| MOTA | 19968 | | TAW | 3038 | 10.453 | 7.434 | 47.450 | 1.00 13.74 |
| ATOM | 19969 | | TAW | 3039 | 0.953 | -32.769 | 9.383 | 1.00 15.20 |
| ATOM | 19970 | | WAT | 3040 | -7.328 | | -18.137 | 1.00 18.80 |
| MOTA | 19971 | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3041 | -8.835 | 2.730 | 43.501 | 1.00 10.87 |
| | | | | | | | | |

| ATOM | 19972 | он2 | WAT | 3042 | -1.580 | -10.794 | 33.592 | 1.00 | 12.62 |
|--------------|----------------|------|----------------------------------|------|----------|---------|---------|------|-------|
| ATOM | 19973 | он2 | | 3043 | -12.914 | -8.541 | 27.617 | 1.00 | 12.73 |
| ATOM | 19974 | OH2 | | 3044 | 21.710 | 13.409 | 25.403 | 1.00 | 31.57 |
| ATOM | 19975 | OH2 | | 3045 | 7.683 | -20.302 | 30.445 | 1.00 | |
| ATOM | 19976 | OH2 | | 3046 | 1.102 | -30.671 | 18.260 | 1.00 | 15.68 |
| | 19977 | OH2 | | 3047 | 28.173 | 7.798 | 31.821 | 1.00 | 20.07 |
| ATOM | | | | 3048 | -1.179 | | 31.883 | | 13.42 |
| ATOM | 19978 | OH2 | | | | | | | 20.69 |
| MOTA | 19979 | OH2 | | 3049 | 13.221 | 14.116 | 19.297 | | |
| MOTA | 19980 | OH2 | | 3050 | -2.044 | 20.189 | 37.466 | | 16.68 |
| MOTA | 19981 | OH2 | | 3051 | . 17.876 | | 39.307 | | 16.30 |
| MOTA | 19982 | он2 | | 3052 | -0.744 | -30.549 | 20.671 | | 17.77 |
| MOTA | 19983 | он2 | | 3053 | 35.481 | | 29.142 | 1.00 | 12.21 |
| ATOM | 19984 | OH2 | | 3054 | -9.507 | | -12.790 | | 16.79 |
| MOTA | 19985 | OH2 | WAT | 3055 | 31.604 | -1.451 | 46.191 | | 14.27 |
| MOTA | 19986 | OH2 | WAT | 3056 | -14.406 | 5.407 | 38.561 | 1.00 | 16.53 |
| ATOM | 19987 | OH2 | TAW | 3057 | -0.928 | -11.952 | 36.038 | | 12.23 |
| ATOM | 19988 | OH2 | WAT | 3058 | 0.468 | -17.148 | 54.501 | 1.00 | 17.45 |
| ATOM | 19989 | OH2 | WAT | 3059 | 5.125 | -36.602 | 35.570 | 1.00 | 20.20 |
| ATOM | 19990 | OH2 | WAT | 3060 | 0.620 | -51.357 | 23.066 | 1.00 | 14.88 |
| ATOM | 19991 | OH2 | WAT | 3061 | 17.818 | -20.565 | 43.493 | 1.00 | 14.36 |
| ATOM | 19992 | он2 | | 3062 | 23.320 | 7.615 | 14.657 | 1.00 | 12.79 |
| ATOM | 19993 | OH2 | | 3063 | -13.311 | 2.901 | 39.033 | 1.00 | 16.11 |
| ATOM | 19994 | OH2 | | 3064 | 32.528 | | 23.589 | 1.00 | 13.88 |
| ATOM . | 19995 | OH2 | | 3065 | 13.191 | -4.951 | 48.336 | 1.00 | 19.12 |
| ATOM | 19996 | OH2 | | 3066 | -11.736 | 7.247 | 3.147 | | 13.94 |
| ATOM | 19997 | OH2 | | 3067 | 32.586 | -0.717 | 43.888 | | 14.86 |
| ATOM | 19998 | OH2 | | 3068 | 11.327 | 19.214 | 30.461 | | 15.85 |
| | | OH2 | | 3069 | 19.105 | | 17.671 | | 11.69 |
| MOTA | 19999 | OH2 | | 3070 | -9.957 | -7.454 | 6.721 | | 17.25 |
| MOTA | 20000 | | | | 9.085 | | 57.247 | | 14.59 |
| ATOM | 20001 | OH2 | | 3071 | | | 24.588 | | 19.14 |
| ATOM | 20002 | OH2 | | 3072 | 39.426 | 3.322 | | | 15.75 |
| MOTA | 20003 | OH2 | | 3073 | 3.530 | 9.016 | 39.444 | | |
| MOTA | 20004 | OH2 | | 3074 | -10.708 | 15.943 | -14.582 | | 14.94 |
| MOTA | 20005 | он2 | | 3075 | -0.027 | | 29.261 | | 12.27 |
| | 20006 | OH2 | | 3076 | 14.927 | -5.859 | -4.822 | | 16.81 |
| MOTA | 20007 | OH2 | | 3077 | -6.247 | 19.997 | 21.778 | | 16.82 |
| MOTA | 20008 | OH2 | | 3078 | 23.194 | -3.748 | 41.708 | | 13.63 |
| MOTA | 20009 | OH2 | | 3079 | 3.044 | -14.551 | 15.690 | | 11.83 |
| MOTA | 20010 | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3080 | | -44.437 | 15.495 | | 16.34 |
| MOTA | 20011 | OH2 | TAW | 3081 | 2.658 | -6.744 | 11.642 | 1.00 | 13.95 |
| ATOM | 20012 | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3082 | 18.097 | -3.425 | 45.902 | 1.00 | 14.60 |
| MOTA | 20013 | OH2 | TAW | 3083 | 17.808 | -10.614 | 17.279 | 1.00 | 20.73 |
| ATOM | 20014 | OH2 | WAT | 3084 | 17.717 | -23.621 | 16.919 | 1.00 | 14.50 |
| ATOM | 20015 | OH2 | WAT | 3085 | 20.450 | -28.027 | 39.405 | 1.00 | 20.21 |
| MOTA | 20016 | OH2 | WAT | 3086 | -16.370 | 8.639 | 40.975 | 1.00 | 19.28 |
| MOTA | 20017 | OH2 | WAT | 3087 | 25.222 | -0.313 | 11.241 | 1.00 | 15.89 |
| ATOM | 20018 | OH2 | TAW | 3088 | 11.033 | -3.025 | -5.467 | 1.00 | 16.78 |
| ATOM | 20019 | | WAT | 3089 | -2.490 | -3.684 | 17.486 | 1.00 | 14.21 |
| ATOM | 20020 | OH2 | TAW | 3090 | 22.173 | -49.823 | 28.580 | 1.00 | 17.88 |
| ATOM | 20021 | | WAT | 3091 | | -16.320 | 27.976 | 1.00 | 15.29 |
| ATOM | 20022 | | WAT | 3092 | -19.387 | | 23.319 | | 14.53 |
| ATOM | 20023 | OH2 | | 3093 | | -8.958 | 15.354 | | 16.00 |
| ATOM | 20023 | | WAT | 3094 | -10.894 | 6.982 | 14.192 | | 14.83 |
| ATOM | 20025 | | WAT | 3095 | 38.364 | | 14.395 | | 14.78 |
| MOTA | 20026 | | WAT | 3096 | -14.355 | | 12.720 | | 16.02 |
| ATOM | 20027 | | WAT | 3097 | -2.640 | | 6.218 | | 14.25 |
| ATOM | 20028 | | WAT | 3098 | 14.236 | | 34.025 | | 14.37 |
| MOTA | 20029 | | WAT | 3099 | -6.286 | | 35.017 | | 17.92 |
| MOTA | 20025 | | WAT | 3100 | 5.618 | | 19.599 | | 18.87 |
| ATOM | 20030 | | WAT | 3101 | 24.798 | | 34.734 | | 20.61 |
| | | | | | 18.157 | | 22.944 | | 18.26 |
| ATOM | 20032 | | WAT | 3102 | 3.448 | | | | 16.83 |
| ATOM | 20033 | | TAW | 3103 | | | 28.656 | | 13.63 |
| ATOM | 20034 | | WAT | 3104 | 37.310 | | 60.707 | | |
| MOTA | 20035 | | WAT | 3105 | 7.399 | | 14.456 | | 15.32 |
| ATOM | 20036 | | WAT | 3106 | -4.065 | | 32.716 | | 13.85 |
| MOTA | 20037 | | TAW | 3107 | 26.681 | | 6.361 | | 16.84 |
| ATOM | 20038 | | WAT | 3108 | 2.621 | | 20.371 | | 18.02 |
| ATOM | 20039 | | WAT | 3109 | -8.257 | | -15.506 | | 17.18 |
| MOTA | 20040 | | WAT | 3110 | -5.408 | | -13.054 | | 16.87 |
| ATOM | 20041 | | WAT | 3111 | -14.226 | | 35.035 | | 19.49 |
| MOTA | 20042 | | TAW | 3112 | 8.844 | | 14.940 | | 13.32 |
| ATOM | 20043 | | WAT | 3113 | 10.416 | | 8.580 | | 19.28 |
| MOTA | 20044 | | WAT | 3114 | 24.321 | | 39.443 | | 14.51 |
| MOTA | 20045 | | WAT | 3115 | 32.620 | | 10.966 | | 18.64 |
| ATOM | 20046 | | WAT | 3116 | 21.077 | | 16.352 | | 16.09 |
| 3 00034 | | 0110 | TAT A TT | 3117 | 11.416 | 8.982 | 43.352 | 1.00 | 19.27 |
| MOTA MOTA | 20047 20048 | OH2 | WAT | 3118 | | -10.327 | 4.606 | | 17.92 |

| ATOM | 20049 | OH2 WAT | 3119 | 11.474 7 | .062 8.572 | 1.00 18.56 |
|------------------------------|----------------------------------|-------------------------------|----------------------|---|--|--|
| ATOM | 20050 | OH2 WAT | 3120 | 17.899 -18 | | |
| | 20051 | OH2 WAT | 3121 | | .445 -5.210 | |
| ATOM | | | | | | |
| MOTA | 20052 | OH2 WAT | 3122 | | .783 40.687 | |
| MOTA | 20053 | OH2 WAT | 3123 | 30.129 -21 | | |
| MOTA | 20054 | OH2 WAT | 3124 | 15.046 -43 | .858 18.014 | 1.00 11.77 |
| ATOM | 20055 | OH2 WAT | 3125 | -9.121 2 | .705 47.977 | 1.00 17.81 |
| ATOM | 20056 | OH2 WAT | 3126 | 34.332 -14 | .474 60.657 | 1.00 24.94 |
| ATOM | 20057 | OH2 WAT | 3127 | | .667 55.823 | 1.00 21.51 |
| ATOM | 20058 | OH2 WAT | 3128 | 33.157 -10 | | |
| | | | | | .084 29.393 | |
| ATOM | 20059 | OH2 WAT | 3129 | | | |
| MOTA | 20060 | OH2 WAT | 3130 | 7.739 -10 | | |
| ATOM | 20061 | OH2 WAT | 3131 | -2.901 -28 | | |
| ATOM | 20062 | OH2 WAT | 3132 | 8.775 -17 | .442 26.955 | 1.00 15.53 |
| MOTA | 20063 | OH2 WAT | 3133 | 10.635 -14 | .815 5.424 | 1.00 17.26 |
| ATOM | 20064 | OH2 WAT | 3134 | -1.407 15 | .539 35.202 | 1.00 21.03 |
| ATOM | 20065 | OH2 WAT | 3135 | 22.262 -3 | .590 54.476 | 1.00 17.12 |
| ATOM | 20066 | OH2 WAT | 3136 | -13.401 -21 | | |
| | | OH2 WAT | 3137 | | .847 47.443 | |
| ATOM | 20067 | | | | | |
| ATOM | 20068 | OH2 WAT | 3138 | | .485 24.661 | |
| MOTA | 20069 | OH2 WAT | 3139 | -2.531 -40 | | |
| MOTA | 20070 | OH2 WAT | 3140 | -1.909 -4 | .892 36.246 | 1.00 16.91 |
| ATOM | 20071 | OH2 WAT | 3141 | -19.604 14 | .972 6.233 | 1.00 20.13 |
| ATOM | 20072 | OH2 WAT | 3142 | -6.017 -42 | .085 21.509 | 1.00 16.39 |
| ATOM | 20073 | OH2 WAT | 3143 | | .282 -13.491 | 1.00 17.83 |
| ATOM | 20074 | OH2 WAT | 3144 | | .827 44.434 | |
| | | OH2 WAT | | | .400 35.274 | |
| ATOM | 20075 | | 3145 | | | |
| ATOM | 20076 | OH2 WAT | 3146 | | | 1.00-13.66 |
| ATOM | 20077 | OH2 WAT | 3147 | | .904 38.629 | |
| MOTA | 20078 | OH2 WAT | 3148 | 5.189 16 | .665 30.863 | 1.00 16.04 |
| ATOM | 20079 | OH2 WAT | 3149 | 8.219 -17 | .924 40.764 | 1.00 16.89 |
| ATOM | 20080 | OH2 WAT | 3150 | 41.387 -1 | .649 40.145 | 1.00 18.07 |
| ATOM | 20081 | OH2 WAT | 3151 | -3.245 -39 | .921 9.833 | 1.00 18.23 |
| ATOM | 20082 | OH2 WAT | 3152 | | .770 11.939 | |
| | 20082 | | . 3153 | | .554 15.618 | |
| ATOM | | | | | | |
| ATOM | 20084 | OH2 WAT | 3154 | 11.910 -17 | | |
| ATOM | 20085 | OH2 WAT | 3155 | -20.114 -12 | | |
| ATOM | 20086 | OH2 WAT | 3156 | -1.281 -11 | .060 5.278 | |
| ATOM | 20087 | OH2 WAT | 3157 | -17.431 3 | .089 39.729 | 1.00 12.26 |
| MOTA | 20088 | OH2 WAT | 3158 | -3.548 -35 | .710 27.746 | 1.00 16.68 |
| ATOM | 20089 | OH2 WAT | 3159 | -17.120 5 | .018 37.848 | 1.00 16.94 |
| ATOM | 20090 | OH2 WAT | 3160 | | .627 54.843 | 1.00 18.64 |
| ATOM | 20091 | OH2 WAT | 3161 | | .014 23.849 | |
| | | | | -13.199 -10 | | |
| MOTA | 20092 | OH2 WAT | 3162 | | | |
| MOTA | 20093 | OH2 WAT | 3163 | | .977 54.316 | |
| ATOM | 20094 | OH2 WAT | 3164 | | .599 61.802 | |
| MOTA | 20095 | OH2 WAT | 3165 | | .982 44.938 | 1.00 17.95 |
| ATOM | 20096 | OH2 WAT | 3166 | 16.321 -50 | .335 21.944 | 1.00 14.95 |
| ATOM | 20097 | OH2 WAT | 3167 | 4.185 -10 | | 1.00 18.49 |
| ATOM | 20098 | OH2 WAT | 3168 | -6.542 2 | .530 38.971 | 1.00 18.82 |
| ATOM | 20099 | OH2 WAT | 3169 | | .493 11.385 | |
| ATOM | | OH2 WAT | 3170 | | | 1.00 15.06 |
| | | | | | | |
| ATOM | 20101 | OH2 WAT | 3171 | | .374 52.309 | |
| ATOM | 20102 | OH2 WAT | 3172 | | .626 63.159 | |
| MOTA | 20103 | OH2 WAT | 3173 | | .987 47.799 | |
| MOTA | 20104 | OH2 WAT | 3174 | | .921 45.943 | |
| MOTA | 20105 | OH2 WAT | 3175 | 4.737 -16 | .653 43.656 | 1.00 23.24 |
| MOTA | 20106 | OH2 WAT | 3176 | 19.671 -2 | .177 44.183 | 1.00 15.91 |
| ATOM | 20107 | OH2 WAT | 3177 | | .921 9.302 | |
| ATOM | 20108 | OH2 WAT | 3178 | 25.798 -18 | | |
| ATOM | 20100 | OH2 WAT | 3179 | | .361 49.300 | |
| | | | 3179 | | | |
| ATOM | 20110 | OH2 WAT | | | | |
| ATOM | 20111 | OH2 WAT | 3181 | | .686 38.364 | |
| ATOM | 20112 | OH2 WAT | 3182 | | .303 53.961 | |
| ATOM | 20113 | OH2 WAT | 3183 | -19.721 -30 | | |
| MOTA | 20114 | OH2 WAT | 3184 | | .768 70.046 | |
| ATOM | 20115 | OH2 WAT | 3185 | 13.397 11 | .894 3.881 | 1.00 22.84 |
| ATOM | 20116 | OH2 WAT | 3186 | | .413 11.054 | 1.00 18.87 |
| ATOM | 20117 | OH2 WAT | 3187 | | .237 -13.520 | |
| ATOM | 20118 | OH2 WAT | 3188 | | .845 48.990 | |
| | | OH2 WAT | 3189 | | .199 37.473 | |
| | 20110 | VOS WAT | | | .973 16.658 | |
| ATOM | 20119 | | | 3 340 10 | | |
| MOTA | 20120 | OH2 WAT | 3190 | | | |
| MOTA MOTA | 20120 20121 | OH2 WAT OH2 WAT | 3191 | -1.268 0 | .118 45.115 | 1.00 20.12 |
| MOTA MOTA MOTA | 20120 20121 20122 | OH2 WAT OH2 WAT OH2 WAT | 3191 3192 | -1.268 0 8.866 - 56 | .118 45.115 .007 22.359 | 1.00 20.12 1.00 22.50 |
| ATOM ATOM ATOM ATOM | 20120 20121 20122 20123 | OH2 WAT OH2 WAT OH2 WAT | 3191 3192 3193 | -1.268 0 8.866 -56 4.755 11 | .118 45.115 .007 22.359 .704 -21.103 | 1.00 20.12 1.00 22.50 1.00 21.21 |
| MOTA MOTA MOTA | 20120 20121 20122 | OH2 WAT OH2 WAT OH2 WAT | 3191 3192 | -1.268 0 8.866 -56 4.755 11 29.496 7 | .118 45.115 .007 22.359 .704 -21.103 .747 5.130 | 1.00 20.12 1.00 22.50 1.00 21.21 1.00 24.25 |
| ATOM ATOM ATOM ATOM | 20120 20121 20122 20123 | OH2 WAT OH2 WAT OH2 WAT | 3191 3192 3193 | -1.268 0 8.866 -56 4.755 11 29.496 7 | .118 45.115 .007 22.359 .704 -21.103 | 1.00 20.12 1.00 22.50 1.00 21.21 1.00 24.25 |

| ATOM | 20126 | OH2 | WAT | 3196 | 6.422 | 15.829 | 26.439 | 1.00 19.29 |
|--------|-------|-----|----------------------------------|------|---------|---------|---------|------------|
| ATOM | 20127 | | WAT | 3197 | | -11.050 | 64.371 | 1.00 18.77 |
| | 20127 | | WAT | 3198 | | -13.631 | 20.195 | 1.00 16.50 |
| ATOM | | | | 3199 | _ | -27.216 | 36.881 | 1.00 18.17 |
| ATOM | 20129 | | WAT | | | -16.462 | 40.801 | 1.00 10.17 |
| ATOM | 20130 | | TAW | 3200 | | | | |
| ATOM | 20131 | | WAT | 3201 | 19.084 | | 46.456 | 1.00 19.77 |
| MOTA | 20132 | | WAT | 3202 | | -21.751 | 8.937 | 1.00 19.12 |
| MOTA | 20133 | | WAT | 3203 | 30.258 | | 39.421 | 1.00 23.25 |
| MOTA | 20134 | | WAT | 3204 | | -46.203 | 12.674 | 1.00 18.08 |
| ATOM | 20135 | | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3205 | -10.806 | | 22.314 | 1.00 22.59 |
| MOTA | 20136 | OH2 | \mathbf{WAT} | 3206 | 25.446 | | 4.362 | 1.00 22.71 |
| MOTA | 20137 | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3207 | -1.437 | -43.569 | 11.596 | 1.00 14.68 |
| ATOM | 20138 | OH2 | WAT | 3208 | 6.165 | 17.099 | 16.294 | 1.00 19.35 |
| MOTA | 20139 | OH2 | WAT | 3209 | 0.456 | -5.728 | 18.027 | 1.00 16.11 |
| ATOM | 20140 | OH2 | WAT | 3210 | 17.554 | -15.937 | 28.233 | 1.00 15.55 |
| ATOM | 20141 | OH2 | WAT | 3211 | 2.388 | -14.201 | 39.957 | 1.00 16.30 |
| MOTA | 20142 | он2 | WAT | 3212 | -8.445 | -43.392 | 21.151 | 1.00 15.83 |
| MOTA | 20143 | | WAT | 3213 | -1.149 | -2.138 | 11.071 | 1.00 16.20 |
| ATOM | 20144 | | WAT | 3214 | | -18.966 | 9.491 | 1.00 22.11 |
| ATOM | 20145 | | WAT | 3215 | 40.917 | | 61.223 | 1.00 17.97 |
| ATOM | 20146 | | WAT | 3216 | 20.418 | | 40.411 | 1.00 18.22 |
| ATOM | 20147 | | WAT | 3217 | 7.210 | | -23.993 | 1.00 22.59 |
| | 20147 | | WAT | 3218 | 13.270 | | -5.622 | 1.00 17.55 |
| ATOM | | | | | | | 65.086 | 1.00 17.33 |
| ATOM | 20149 | | WAT | 3219 | 16.193 | | 53.690 | 1.00 23.17 |
| MOTA | 20150 | | WAT | 3220 | 1.345 | | | 1.00 19.22 |
| MOTA | 20151 | | TAW | 3221 | | -28.861 | 12.302 | |
| MOTA | 20152 | | TAW | 3222 | -5.861 | | 53.062 | 1.00 22.85 |
| MOTA | 20153 | | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3223 | | -17.385 | 9.566 | 1.00 14.82 |
| MOTA | 20154 | | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3224 | 5.907 | | 37.560 | 1.00 23.71 |
| ATOM | 20155 | | TAW | 3225 | 9.404 | | -17.364 | 1.00 18.51 |
| MOTA | 20156 | он2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3226 | -19.508 | 18.345 | -4.134 | 1.00 18.87 |
| MOTA | 20157 | OH2 | WAT | 3227 | 43.927 | 19.766 | 59.453 | 1.00 22.41 |
| ATOM | 20158 | он2 | TAW | 3228 | 10.197 | 3.381 | 10.668 | 1.00 16.51 |
| MOTA | 20159 | OH2 | WAT | 3229 | -14.378 | 18.764 | 53.775 | 1.00 20.79 |
| MOTA | 20160 | OH2 | WAT | 3230 | -20.438 | -16.179 | 61.040 | 1.00 22.89 |
| MOTA | 20161 | OH2 | WAT | 3231 | 30.282 | -36.634 | 32.910 | 1.00 15.84 |
| MOTA | 20162 | он2 | WAT | 3232 | 39.788 | 13.875 | 64.578 | 1.00 17.48 |
| ATOM | 20163 | | WAT | 3233 | -21.813 | -14.345 | 7.149 | 1.00 19.96 |
| ATOM | 20164 | | WAT | 3234 | | -16.263 | 23.755 | 1.00 24.36 |
| ATOM | 20165 | | WAT | 3235 | 32.740 | | 50.333 | 1.00 19.77 |
| ATOM | 20166 | | WAT | 3236 | | -40.590 | 22.042 | 1.00 15.97 |
| ATOM | 20167 | | WAT | 3237 | -20.321 | | 29.261 | 1.00 17.79 |
| ATOM | 20168 | | WAT | 3238 | | -16.348 | 54.593 | 1.00 23.74 |
| ATOM | 20169 | | WAT | 3239 | 32.211 | | 12.342 | 1.00 12.74 |
| ATOM | 20170 | | WAT | 3240 | | -38.308 | 33.861 | 1.00 27.01 |
| | 20170 | | WAT | 3241 | -5.435 | | 15.587 | 1.00 27.61 |
| ATOM | | | | | 5.162 | • | 9.145 | 1.00 25.66 |
| MOTA | 20172 | | WAT | 3242 | -12.976 | | 1.055 | 1.00 15.00 |
| ATOM | 20173 | | WAT | 3243 | | | | |
| MOTA | 20174 | | WAT | 3244 | | -50.548 | 27.523 | 1.00 18.25 |
| MOTA | 20175 | | TAW | 3245 | 23.502 | | 17.712 | 1.00 21.76 |
| MOTA | 20176 | | TAW | 3246 | 29.781 | | -12.106 | 1.00 22.34 |
| MOTA | 20177 | | WAT | 3247 | 16.179 | | | 1.00 17.27 |
| MOTA | 20178 | | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3248 | 25.630 | | 35.873 | 1.00 24.47 |
| ATOM | 20179 | | WAT | 3249 | 19.075 | | 8.867 | 1.00 17.88 |
| MOTA | 20180 | | TAW | 3250 | 24.463 | | 55.349 | 1.00 19.50 |
| MOTA | 20181 | | WAT | 3251 | 6.006 | | 8.134 | 1.00 18.83 |
| MOTA | 20182 | | WAT | 3252 | | -22.682 | 41.765 | 1.00 22.36 |
| ATOM | 20183 | OH2 | WAT | 3253 | -14.877 | | 15.278 | 1.00 19.04 |
| ATOM | 20184 | OH2 | WAT | 3254 | 6.808 | | 49.732 | 1.00 18.14 |
| MOTA | 20185 | OH2 | \mathbf{WAT} | 3255 | 26.166 | 5.603 | 20.868 | 1.00 21.17 |
| MOTA | 20186 | OH2 | WAT | 3256 | 4.305 | -15.545 | 56.992 | 1.00 16.97 |
| ATOM | 20187 | OH2 | TAW | 3257 | 13.421 | -15.839 | 15.404 | 1.00 19.34 |
| MOTA | 20188 | OH2 | WAT | 3258 | -12.696 | -19.398 | 26.900 | 1.00 26.15 |
| ATOM | 20189 | OH2 | WAT | 3259 | 5.047 | -18.352 | 55.566 | 1.00 20.95 |
| ATOM | 20190 | OH2 | WAT | 3260 | -21.140 | -30.966 | 20.114 | 1.00 22.15 |
| ATOM | 20191 | OH2 | WAT | 3261 | -0.778 | 32.093 | 65.599 | 1.00 22.89 |
| ATOM | 20192 | | WAT | 3262 | | -12.190 | 8.019 | 1.00 19.08 |
| ATOM | 20193 | | WAT | 3263 | -9.797 | | -14.744 | 1.00 15.93 |
| ATOM | 20194 | | WAT | 3264 | -6.689 | | 46.121 | 1.00 15.64 |
| ATOM | 20195 | | WAT | 3265 | 14.061 | | 42.176 | 1.00 31.75 |
| ATOM | 20196 | | WAT | 3266 | -0.527 | | 42.399 | 1.00 20.09 |
| ATOM | 20197 | | WAT | 3267 | -0.194 | | 58.037 | 1.00 23.96 |
| ATOM | 20197 | | WAT | 3268 | | -17.073 | 22.925 | 1.00 20.92 |
| ATOM | 20198 | | WAT | 3269 | 41.330 | | 15.013 | 1.00 20.32 |
| ATOM | 20200 | | WAT | 3270 | 4.620 | | -6.543 | 1.00 23.33 |
| MOTA | 20200 | | WAT | 3270 | | -17.451 | 41.068 | 1.00 24.77 |
| ATOM | 20201 | | WAT | 3272 | 25.285 | | 32.566 | 1.00 18.93 |
| A I OH | 20202 | Onz | AAS-7 T | 3616 | 45.465 | 11.402 | 32.300 | 1.00 13.14 |

| ATOM | 20203 | OH2 WAT | 3273 | 41.753 | -19.624 | 48.472 | 1.00 23.10 |
|--------------|-------|----------|------|---------|----------------|---------|------------|
| MOTA | 20204 | OH2 WAT | 3274 | 4.615 | 0.859 | 46.531 | 1.00 16.54 |
| ATOM | 20205 | OH2 WAT | 3275 | 31.542 | -15.777 | 28.303 | 1.00 20.38 |
| ATOM | 20206 | OH2 WAT | 3276 | 19.527 | 11.849 | 39.254 | 1.00 15.70 |
| | 20207 | OH2 WAT | 3277 | 33.147 | -23.760 | 25.248 | 1.00 16.58 |
| MOTA | | | | | • | | 1.00 29.58 |
| MOTA | 20208 | OH2 WAT | 3278 | | -49.095 | 13.770 | |
| ATOM | 20209 | OH2 WAT | 3279 | 23.794 | -15.430 | 33.966 | 1.00 21.14 |
| ATOM | 20210 | OH2 WAT | 3280 | -14.122 | 0.241 | -14.020 | 1.00 21.60 |
| MOTA | 20211 | OH2 WAT | 3281 | -31.126 | -7.465 | 48.968 | 1.00 18.37 |
| ATOM | 20212 | OH2 WAT | 3282 | 33.182 | 4.867 | 26.769 | 1.00 29.67 |
| | | | | | | 32.613 | 1.00 23.60 |
| ATOM | 20213 | OH2 WAT | 3283 | 24.781 | 8.897 | | |
| ATOM | 20214 | OH2 WAT | 3284 | 37.324 | -32.782 | 27.936 | 1.00 20.55 |
| MOTA | 20215 | OH2 WAT | 3285 | 36.703 | -2.932 | 24.810 | 1.00 20.31 |
| MOTA | 20216 | OH2 WAT | 3286 | 16.737 | 6.043 | -10.203 | 1.00 14.77 |
| ATOM | 20217 | OH2 WAT | 3287 | 42.281 | 10.193 | 65.227 | 1.00 20.86 |
| ATOM | 20218 | OH2 WAT | 3288 | -24.643 | -24.852 | 6.883 | 1.00 22.27 |
| | | | | 3.427 | 33.777 | 58.006 | 1.00 17.87 |
| MOTA | 20219 | OH2 WAT | 3289 | | | | |
| MOTA | 20220 | OH2 WAT | 3290 | 26.392 | 2.408 | 17.399 | 1.00 19.04 |
| MOTA | 20221 | OH2 WAT | 3291 | -18.654 | -5.950 | 66.016 | 1.00 23.24 |
| MOTA | 20222 | OH2 WAT | 3292 | -13.093 | -15.210 | 22.791 | 1.00 20.23 |
| ATOM | 20223 | OH2 WAT | 3293 | 9.173 | -6.311 | 51.088 | 1.00 24.64 |
| ATOM | 20224 | OH2 WAT | 3294 | | -37.037 | 23.715 | 1.00 17.22 |
| | | | | | -28.491 | 18.445 | 1.00 21.94 |
| ATOM | 20225 | OH2 WAT | 3295 | -23.611 | | | |
| MOTA | 20226 | OH2 WAT | 3296 | | -20.767 | 2.623 | 1.00 21.92 |
| MOTA | 20227 | OH2 WAT | 3297 | 5.370 | -10.917 | 64.991 | 1.00 20.49 |
| ATOM | 20228 | OH2 WAT | 3298 | 21.104 | 12.701 | 14.311 | 1.00 20.74 |
| ATOM | 20229 | OH2 WAT | 3299 | -8.121 | 27.589 | 65.671 | 1.00 30.46 |
| ATOM | 20230 | OH2 WAT | 3300 | 17.972 | 5.158 | 7.455 | 1.00 16.91 |
| | | OH2 WAT | 3301 | 10.494 | -0.984 | -3.411 | 1.00 21.18 |
| MOTA | 20231 | | | | | | |
| MOTA | 20232 | OH2 WAT | 3302 | 4.032 | 42.243 | 10.424 | 1.00 30.91 |
| ATOM | 20233 | OH2 WAT | 3303 | 24.441 | -27.550 | 68.904 | 1.00 18.25 |
| MOTA | 20234 | OH2 WAT | 3304 | 6.219 | 21.783 | 14.079 | 1.00 25.97 |
| MOTA | 20235 | OH2 WAT | 3305 | 23.593 | -1.831 | 13.125 | 1.00 19.74 |
| ATOM | 20236 | OH2 WAT | 3306 | -17.736 | 1.565 | 54.302 | 1.00 19.29 |
| | | OH2 WAT | 3307 | 13.850 | -2.899 | -3.293 | 1.00 22.15 |
| MOTA | 20237 | | | | | | |
| MOTA | 20238 | OH2 WAT | 3308 | 34.332 | -43.289 | 29.457 | 1.00 20.15 |
| MOTA | 20239 | OH2 WAT | 3309 | -5.197 | -6.814 | 1.773 | 1.00 19.55 |
| MOTA | 20240 | OH2 WAT | 3310 | -12.090 | 18.072 | 36.228 | 1.00 19.58 |
| MOTA | 20241 | OH2 WAT | 3311 | 17.354 | 10.254 | 43.120 | 1.00 34.77 |
| ATOM | 20242 | OH2 WAT | 3312 | -3.313 | 11.757 | 19.670 | 1.00 26.41 |
| ATOM | 20243 | OH2 WAT | 3313 | 8.528 | -13.751 | 41.287 | 1.00 21.05 |
| | | | | 0.520 | | | |
| MOTA | 20244 | OH2 WAT | 3314 | 32.008 | -20.113 | 6.850 | 1.00 25.55 |
| MOTA | 20245 | OH2 WAT | 3315 | 13.281 | 16.160 | 15.117 | 1.00 24.88 |
| MOTA | 20246 | OH2. WAT | 3316 | 28.691 | 9.379 | 7.117 | 1.00 20.59 |
| MOTA | 20247 | OH2 WAT | 3317 | 23.789 | -6.461 | 61.180 | 1.00 26.68 |
| MOTA | 20248 | OH2 WAT | 3318 | 1.515 | 36.096 | 58.072 | 1.00 18.91 |
| ATOM | 20249 | OH2 WAT | 3319 | 48.872 | 11.459 | 42.531 | 1.00 27.53 |
| | | OH2 WAT | | 5.225 | -25.223 | 34.596 | 1.00 14.92 |
| MOTA | 20250 | | 3320 | | | | |
| ATOM | 20251 | OH2 WAT | 3321 | 37.106 | -22.432 | 3.847 | 1.00 17.63 |
| ATOM | 20252 | OH2 WAT | 3322 | -9.345 | -4.853 | 27.183 | 1.00 24.67 |
| ATOM | 20253 | OH2 WAT | 3323 | 34.721 | -21.213 | 36.495 | 1.00 21.39 |
| ATOM | 20254 | OH2 WAT | 3324 | 32.652 | -14.927 | -13.607 | 1.00 25.32 |
| ATOM | 20255 | OH2 WAT | 3325 | -13.339 | 21.021 | -8.922 | 1.00 22.80 |
| MOTA | 20256 | OH2 WAT | 3326 | -3.296 | -1.036 | 16.162 | 1.00 24.45 |
| | | | | | | | 1.00 23.66 |
| MOTA | 20257 | OH2 WAT | 3327 | 9.522 | -32.401 | 16.459 | |
| MOTA | 20258 | OH2 WAT | 3328 | 18.151 | 15.055 | 63.606 | 1.00 19.05 |
| MOTA | 20259 | OH2 WAT | 3329 | | -47.125 | 10.644 | 1.00 21.08 |
| ATOM | 20260 | OH2 WAT | 3330 | -9.192 | 11.917 | 33.840 | 1.00 20.79 |
| MOTA | 20261 | OH2 WAT | 3331 | 4.631 | -19.143 | 15.726 | 1.00 20.59 |
| ATOM | 20262 | OH2 WAT | 3332 | 18.911 | 18.491 | 41.568 | 1.00 24.07 |
| ATOM | 20262 | OH2 WAT | 3333 | -17.813 | 22.262 | 45.797 | 1.00 26.58 |
| | | | | | | | |
| ATOM | 20264 | OH2 WAT | 3334 | | -28.271 | 37.324 | 1.00 25.49 |
| ATOM | 20265 | OH2 WAT | 3335 | 29.350 | -5.186 | 2.361 | 1.00 31.20 |
| MOTA | 20266 | OH2 WAT | 3336 | 7.196 | -5.221 | 46.352 | 1.00 22.56 |
| MOTA | 20267 | OH2 WAT | 3337 | 54.614 | 10.503 | 48.370 | 1.00 21.87 |
| MOTA | 20268 | OH2 WAT | 3338 | 12.377 | -24.993 | 37.751 | 1.00 21.71 |
| ATOM | 20269 | OH2 WAT | 3339 | 16.863 | 5.321 | 48.931 | 1.00 23.14 |
| | | | | | | | |
| ATOM | 20270 | OH2 WAT | 3340 | -8.724 | 19.145 | 20.888 | 1.00 19.11 |
| MOTA | 20271 | OH2 WAT | 3341 | 13.381 | -19.714 | -4.203 | 1.00 16.96 |
| ATOM | 20272 | OH2 WAT | 3342 | 11.141 | 15.500 | -6.398 | 1.00 25.52 |
| ATOM | 20273 | OH2 WAT | 3343 | -0.771 | 12.885 | 18.816 | 1.00 31.48 |
| MOTA | 20274 | OH2 WAT | 3344 | -16.965 | 4.474 | 14.900 | 1.00 22.48 |
| ATOM | 20275 | OH2 WAT | 3345 | 19.464 | 21.926 | 68.546 | 1.00 24.61 |
| | | | | -8.665 | -0.567 | 10.532 | 1.00 24.01 |
| ATOM | 20276 | OH2 WAT | 3346 | | | | |
| ATOM | | | 3347 | 19.548 | -3.441 | 41.810 | 1.00 18.14 |
| | 20277 | OH2 WAT | | | | | |
| MOTA | 20278 | OH2 WAT | 3348 | 3.984 | 5.093 | 41.179 | 1.00 19.65 |
| ATOM ATOM | | | | | 5.093 4.713 | | |

| MOTA | 20280 | OH2 WAT | 3350 | 9.510 | -54.905 | 26.309 | 1.00 22.92 |
|------|-------|---------|------|---------|---------|---------|-------------|
| ATOM | 20281 | OH2 WAT | 3351 | 2.738 | 2.375 | 54.788 | 1.00 21.38 |
| | 20282 | OH2 WAT | 3352 | 38.200 | -3.877 | 39.235 | 1.00 17.67 |
| MOTA | | | | | 14.126 | 13.818 | 1.00 21.22 |
| MOTA | 20283 | OH2 WAT | 3353 | 10.728 | | | |
| MOTA | 20284 | OH2 WAT | 3354 | -1.810 | -3.501 | -10.761 | 1.00 32.21 |
| MOTA | 20285 | OH2 WAT | 3355 | 23.131 | 20.084 | 52.484 | 1.00 21.25 |
| ATOM | 20286 | OH2 WAT | 3356 | 13.275 | 37.450 | 61.583 | 1.00 23.72 |
| MOTA | 20287 | OH2 WAT | 3357 | 14.902 | -27.854 | 39.228 | 1.00 17.88 |
| ATOM | 20288 | OH2 WAT | 3358 | 17.196 | 0.708 | -19.731 | 1.00 22.56 |
| ATOM | 20289 | OH2 WAT | 3359 | 12.894 | 27.941 | 72.812 | 1.00 22.10 |
| | 20290 | OH2 WAT | 3360 | 51.803 | 18.337 | 55.429 | 1.00 23.28 |
| MOTA | | | | | | | 1.00 23.20 |
| ATOM | 20291 | OH2 WAT | 3361 | 23.951 | 22.297 | 38.321 | |
| ATOM | 20292 | OH2 WAT | 3362 | 28.231 | 10.502 | 25.782 | 1.00 29.33 |
| MOTA | 20293 | OH2 WAT | 3363 | -19.632 | -10.100 | 40.923 | 1.00 24.00 |
| ATOM | 20294 | OH2 WAT | 3364 | 0.381 | -18.881 | 70.964 | 1.00 24.24 |
| ATOM | 20295 | OH2 WAT | 3365 | 41.050 | -6.012 | 15.791 | 1.00 25.68 |
| MOTA | 20296 | OH2 WAT | 3366 | 25.036 | -21.624 | 17.420 | 1.00 19.61 |
| АТОМ | 20297 | OH2 WAT | 3367 | | -12.469 | 18.162 | 1.00 19.66 |
| ATOM | 20298 | OH2 WAT | 3368 | | -39.595 | 34.156 | 1.00 17.92 |
| | | | | -29.570 | -5.102 | 46.308 | 1.00 22.63 |
| ATOM | 20299 | OH2 WAT | 3369 | | | | |
| ATOM | 20300 | OH2 WAT | 3370 | -4.963 | 11.491 | 58.938 | 1.00 26.60 |
| ATOM | 20301 | OH2 WAT | 3371 | -1.293 | 15.137 | -16.952 | 1.00 22.14 |
| MOTA | 20302 | OH2 WAT | 3372 | 7.371 | 10.814 | 64.052 | 1.00 22.29 |
| MOTA | 20303 | OH2 WAT | 3373 | 16.271 | -27.044 | 44.698 | 1.00 21.59 |
| ATOM | 20304 | OH2 WAT | 3374 | -9.825 | -19.028 | 36.378 | 1.00 15.87 |
| ATOM | 20305 | OH2 WAT | 3375 | -24.137 | -9.482 | 10.270 | 1.00 23.02 |
| MOTA | 20306 | OH2 WAT | 3376 | | -13.121 | 62.268 | 1.00 20.24 |
| | | OH2 WAT | | -11.384 | 0.851 | 7.106 | 1.00 24.50 |
| ATOM | 20307 | | 3377 | | | | |
| MOTA | 20308 | OH2 WAT | 3378 | | -12.471 | 14.199 | 1.00 23.08 |
| ATOM | 20309 | OH2 WAT | 3379 | | -14.517 | 6.808 | 1.00 23.32 |
| MOTA | 20310 | OH2 WAT | 3380 | | -27.767 | 19.798 | 1.00 21.29 |
| MOTA | 20311 | OH2 WAT | 3381 | -0.354 | -4.894 | -20.116 | 1.00 24.42 |
| MOTA | 20312 | OH2 WAT | 3382 | -21.061 | -11.267 | 68.198 | 1.00 30.13 |
| ATOM | 20313 | OH2 WAT | 3383 | -14.706 | -12.293 | 29.188 | 1.00 20.50. |
| ATOM | 20314 | OH2 WAT | 3384 | 43.391 | 2.510 | 23.335 | 1.00 25.76 |
| MOTA | 20315 | OH2 WAT | 3385 | 3.515 | 39.540 | 67.856 | 1.00 26.52 |
| | | | | | | | 1.00 20.32 |
| MOTA | 20316 | OH2 WAT | 3386 | -1.928 | | -25.826 | |
| MOTA | 20317 | OH2 WAT | 3387 | 50.385 | 2.215 | 42.463 | 1.00 29.09 |
| MOTA | 20318 | OH2 WAT | 3388 | 17.087 | 16.878 | 20.716 | 1.00 3,7.71 |
| MOTA | 20319 | OH2 WAT | 3389 | 8.298 | 15.973 | 7.123 | 1.00 32.77 |
| MOTA | 20320 | OH2 WAT | 3390 | 34.661 | -21.425 | 25.109 | 1.00 19.60 |
| ATOM | 20321 | OH2 WAT | 3391 | 19.966 | -51.330 | 15.176 | 1.00 26.16 |
| ATOM | 20322 | OH2 WAT | 3392 | -9.059 | -4.483 | 51.040 | 1.00 20.52 |
| | 20323 | OH2 WAT | 3393 | 25.707 | -32.629 | 33.317 | 1.00 17.81 |
| ATOM | | | | 5.534 | 19.085 | 5.472 | 1.00 33.14 |
| ATOM | 20324 | OH2 WAT | 3394 | | | | |
| MOTA | 20325 | OH2 WAT | 3395 | 14.622 | 19.551 | 55.214 | 1.00 19.96 |
| MOTA | 20326 | OH2 WAT | 3396 | | -14.087 | 20.835 | 1.00 28.72 |
| MOTA | 20327 | OH2 WAT | 3397 | 13.290 | 17.903 | 38.782 | 1.00 20.42 |
| MOTA | 20328 | OH2 WAT | 3398 | -5.862 | -4.263 | 56.954 | 1.00 32.48 |
| MOTA | 20329 | OH2 WAT | 3399 | 6.562 | 15.994 | 19.058 | 1.00 25.19 |
| ATOM | 20330 | OH2 WAT | 3400 | 14.970 | 3.846 | -18.083 | 1.00 19.32 |
| MOTA | 20331 | OH2 WAT | 3401 | -7.124 | 15.004 | -19.783 | 1.00 24.92 |
| MOTA | 20332 | OH2 WAT | 3402 | 34.119 | | -11.775 | 1.00 21.64 |
| | | | | 5.848 | 15.691 | 37.447 | 1.00 21.96 |
| MOTA | 20333 | OH2 WAT | 3403 | | 5.307 | 38.927 | 1.00 28.93 |
| ATOM | 20334 | OH2 WAT | 3404 | -4.384 | | | |
| ATOM | 20335 | OH2 WAT | 3405 | -8.462 | 19.489 | -3.041 | 1.00 23.36 |
| MOTA | 20336 | OH2 WAT | 3406 | 21.504 | -14.699 | 19.950 | 1.00 29.34 |
| MOTA | 20337 | OH2 WAT | 3407 | -21.088 | 4.227 | 39.634 | 1.00 22.61 |
| MOTA | 20338 | OH2 WAT | 3408 | -5.619 | -10.651 | 5.927 | 1.00 24.23 |
| ATOM | 20339 | OH2 WAT | 3409 | 52.693 | 1.167 | 48.206 | 1.00 21.20 |
| MOTA | 20340 | OH2 WAT | 3410 | -16.221 | -9.667 | 65.559 | 1.00 20.52 |
| ATOM | 20341 | OH2 WAT | 3411 | -25.467 | -9.423 | 43.328 | 1.00 24.48 |
| ATOM | 20342 | OH2 WAT | 3412 | -20.988 | 4.741 | 56.477 | 1.00 26.96 |
| ATOM | 20342 | OH2 WAT | 3413 | 19.198 | 18.956 | 55.185 | 1.00 23.07 |
| | | | | | -31.934 | 12.026 | 1.00 25.07 |
| ATOM | 20344 | OH2 WAT | 3414 | -24.253 | | | |
| ATOM | 20345 | OH2 WAT | 3415 | 12.072 | 18.774 | 35.664 | 1.00 23.52 |
| MOTA | 20346 | OH2 WAT | 3416 | -12.454 | 3.743 | 32.390 | 1.00 17.67 |
| ATOM | 20347 | OH2 WAT | 3417 | -18.447 | 6.868 | 40.520 | 1.00 24.96 |
| ATOM | 20348 | OH2 WAT | 3418 | 6.103 | -8.025 | 44.128 | 1.00 27.53 |
| ATOM | 20349 | OH2 WAT | 3419 | -15.120 | -36.912 | 4.961 | 1.00 24.66 |
| ATOM | 20350 | OH2 WAT | 3420 | 18.742 | 5.029 | 46.950 | 1.00 28.56 |
| ATOM | 20351 | OH2 WAT | 3421 | 14.049 | -14.727 | 75.131 | 1.00 22.18 |
| ATOM | 20352 | OH2 WAT | 3422 | 25.532 | -35.284 | 59.886 | 1.00 25.87 |
| MOTA | 20352 | OH2 WAT | 3423 | 14.242 | 4.864 | 4.801 | 1.00 26.11 |
| | | | | | -8.983 | 62.076 | 1.00 23.05 |
| MOTA | 20354 | OH2 WAT | 3424 | 2.505 | | | |
| ATOM | 20355 | OH2 WAT | 3425 | 6.236 | 16.265 | 5.305 | 1.00 24.87 |
| MOTA | 20356 | OH2 WAT | 3426 | 7.628 | -26.541 | 40.424 | 1.00 27.19 |
| | | | | | | | |

| ATOM | 20357 | OH2 WAT | 3427 | 10.084 | 5.888 | 54.362 | 1.00 18.70 |
|----------------------|-------------------------|-------------------------------|--------------|------------------|------------------|-------------------|--------------------------|
| ATOM | 20358 | OH2 WAT | 3428 | -27.669 | -4.824 | 17.585 | 1.00 22.63 |
| | | OH2 WAT | 3429 | 16.131 - | | 20.651 | 1.00 27.80 |
| MOTA | 20359 | | | | | | |
| MOTA | 20360 | OH2 WAT | 3430 | | -10.761 | 21.863 | 1.00 20.66 |
| MOTA | 20361 | OH2 WAT | 3431 | 38.906 | -5.089 | -12.711 | 1.00 32.66 |
| MOTA | 20362 | OH2 WAT | 3432 | 3.036 | 6.220 | 15.329 | 1.00 21.16 |
| ATOM | 20363 | OH2 WAT | 3433 | -5.338 | 0.253 | 17.916 | 1.00 28.50 |
| ATOM | 20364 | OH2 WAT | 3434 | -6.431 | 25.378 | 65.275 | 1.00 28.77 |
| | | | 3435 | | -20.851 | 68.133 | 1.00 27.16 |
| MOTA | 20365 | OH2 WAT | | | | | |
| ATOM | 20366 | OH2 WAT | 3436 | 43.659 | | -1.106 | 1.00 24.34 |
| ATOM | 20367 | OH2 WAT | 3437 | 30.093 | 19.087 | 34.416 | 1.00 35.14 |
| ATOM | 20368 | OH2 WAT | 3438 | -30.035 | -9.535 | 13.285 | 1.00 30.59 |
| ATOM | 20369 | OH2 WAT | 3439 | -17.340 - | -10.617 | 62.281 | 1.00 21.35 |
| ATOM | 20370 | OH2 WAT | 3440 | 4.191 | -8.621 | 64.549 | 1.00 25.99 |
| | 20371 | OH2 WAT | 3441 | 26.000 | -4.755 | 17.793 | 1.00 27.01 |
| MOTA | | | | | | | 1.00 21.29 |
| MOTA | 20372 | OH2 WAT | 3442 | -7.412 | | -20.059 | |
| MOTA | 20373 | OH2 WAT | 3443 | -7.879 | 17.002 | 4.254 | 1.00 26.02 |
| ATOM | 20374 | OH2 WAT | 3444 | -9.087 | -0.369 | 8.012 | 1.00 22.06 |
| MOTA | 20375 | OH2 WAT | 3445 | -23.952 | 1.102 | -9.034 | 1.00 28.67 |
| MOTA | 20376 | OH2 WAT | 3446 | -10.640 | 18.228 | 58.792 | 1.00 24.48 |
| ATOM | 20377 | OH2 WAT | 3447 | -28.943 | 1.338 | 47.872 | 1.00 24.52 |
| | | OH2 WAT | 3448 | | -26.895 | 47.186 | 1.00 25.17 |
| ATOM | 20378 | | | | | | |
| MOTA | 20379 | OH2 WAT | 3449 | -19.226 | 4.149 | 7.394 | |
| ATOM | 20380 | OH2 WAT | 3450 | 16.180 | | 16.613 | 1.00 19.97 |
| MOTA | 20381 | OH2 WAT | 3451 | 7.659 | -6.722 | -19.699 | 1.00 24.66 |
| ATOM | 20382 | OH2 WAT | 3452 | 37.335 | -8.150 | 16.691 | 1.00 18.64 |
| ATOM | 20383 | OH2 WAT | 3453 | 20.745 | 12.571 | 18.819 | 1.00 24.11 |
| | 20384 | | 3454 | -17.203 | -1.956 | 26.377 | 1.00 19.51 |
| MOTA | | | | | | | 1.00 18.81 |
| MOTA | 20385 | OH2 WAT | 3455 | | -15.336 | 31.913 | |
| MOTA | 20386 | OH2 WAT | 3456 | | -48.754 | 10.866 | 1.00 27.33 |
| MOTA | 20387 | OH2 WAT | 3457 | 15.343 | 19.454 | 38.824 | 1.00 23.12 |
| ATOM | 20388 | OH2 WAT | 3458 | 20.577 | -15.545 | 35.392 | 1.00 27.66 |
| ATOM | 20389 | OH2 WAT | 3459 | 41.003 | 1.947 | 26.461 | 1.00 21.44 |
| ATOM | 20390 | OH2 WAT | 3460 | -19.312 | 17.129 | -0.087 | 1.00 24.24 |
| ATOM | 20391 | OH2 WAT | 3461 | 41.814 | | 59.142 | 1.00 29.16 |
| | | | | -23.822 | -2.922 | 29.368 | 1.00 26.46 |
| ATOM | 20392 | OH2 WAT | 3462 | | | | |
| MOTA | 20393 | OH2 WAT | 3463 | -19.777 · | | 63.713 | 1.00 22.86 |
| MOTA | 20394 | OH2 WAT | 3464 | 9.958 | 49.419 | 21.653 | 1.00 31.91 |
| MOTA | 20395 | OH2 WAT | 3465 | -14.397 | 0.840 | 6.887 | 1.00 19.97 |
| ATOM | 20396 | OH2 WAT | 3466 | 41.165 | 1.509 | 54.227 | 1.00 20.56 |
| MOTA | 20397 | OH2 WAT | 3467 | 34.145 | -48.601 | 22.561 | 1.00 23.68 |
| ATOM | 20398 | OH2 WAT | 3468 | 14.133 | | -25.544 | 1.00 32.11 |
| | | | | -1.808 | | 29.404 | 1.00 23.41 |
| MOTA | 20399 | OH2 WAT | | | | | |
| MOTA | 20400 | OH2 WAT | 3470 | | -31.627 | 30.385 | 1.00 31.57 |
| MOTA | 20401 | OH2 WAT | 3471 | 14.985 | -55.814 | 12.662 | 1.00 21.80 |
| MOTA | 20402 | OH2 WAT | 3472 | 24.908 | -25.348 | 43.709 | 1.00 20.59 |
| MOTA | 20403 | OH2 WAT | 3473 | 25.698 | -49.669 | 27.512 | 1.00 22.17 |
| ATOM | 20404 | OH2 WAT | 3474 | 17.811 | -17.127 | 39.808 | 1.00 17.19 |
| ATOM | 20405 | OH2 WAT | 3475 | 21.718 | 14.837 | 7.814 | 1.00 24.90 |
| ATOM | | | 3476 | 22.441 | -3.352 | 58.930 | 1.00 24.81 |
| | 20406 | OH2 WAT | | | | 43.032 | |
| MOTA | 20407 | OH2 WAT | 3477 | 24.448 | 30.315 | | 1.00 26.95 |
| MOTA | 20408 | OH2 WAT | 3478 | 44.123 | 12.038 | 19.936 | 1.00 31.08 |
| MOTA | 20409 | OH2 WAT | 3479 | 20.286 | -30.479 | 61.570 | 1.00 20.29 |
| MOTA | 20410 | OH2 WAT | 3480 | 38.326 | -19.073 | 41.512 | 1.00 22.18 |
| MOTA | 20411 | OH2 WAT | 3481 | -14.815 | 27.992 | 61.688 | 1.00 40.66 |
| ATOM | 20412 | OH2 WAT | 3482 | 34.625 | | 39.822 | 1.00 33.03 |
| ATOM | 20412 | OH2 WAT | 3483 | -3.096 | 35.761 | 7.054 | 1.00 38.60 |
| | | | | | -32.525 | 39.001 | 1.00 30.29 |
| ATOM | 20414 | OH2 WAT | 3484 | | | | |
| MOTA | 20415 | OH2 WAT | 3485 | | -31.893 | 10.831 | 1.00 21.28 |
| MOTA | 20416 | OH2 WAT | 3486 | | -13.200 | | 1.00 28.57 |
| MOTA | 20417 | OH2 WAT | 3487 | 7.504 | 28.777 | 40.806 | 1.00 31.23 |
| MOTA | 20418 | OH2 WAT | 3488 | -9.436 | 22.775 | 21.943 | 1.00 18.82 |
| MOTA | 20419 | OH2 WAT | 3489 | 29.474 | 3.455 | 1.487 | 1.00 32.63 |
| ATOM | 20420 | OH2 WAT | 3490 | 0.602 | 20.241 | 7.100 | 1.00 22.23 |
| | | | | | | 5.724 | 1.00 22.23 |
| ATOM | 20421 | OH2 WAT | 3491 | 9.850 | -7.937 | | |
| ATOM | 20422 | OH2 WAT | 3492 | | -21.034 | | 1.00 30.63 |
| ATOM | 20423 | OH2 WAT | 3493 | 7.930 | | 18.890 | 1.00 20.22 |
| MOTA | 20424 | OH2 WAT | 3494 | -4.506 | -24.196 | 3.635 | 1.00 18.30 |
| ATOM | 20425 | OH2 WAT | 3495 | 10.221 | -19.687 | 36.867 | 1.00 24.52 |
| ATOM | 20426 | OH2 WAT | 3496 | -1.557 | 19.729 | 17.609 | 1.00 19.45 |
| MOTA | 20427 | OH2 WAT | 3497 | -29.812 | -4.805 | 64.317 | 1.00 19.66 |
| | 2042/ | OH2 WAT | 3498 | -26.364 | 8.727 | -2.492 | 1.00 23.78 |
| | 20420 | | ンチスク | | | | 1.00 23.10 |
| ATOM | 20428 | | 2422 | | | E 4 400 | 1 00 26 52 |
| MOTA | 20429 | OH2 WAT | 3499 | | -15.486 | 54.400 | 1.00 26.52 |
| ATOM ATOM | 20429 20430 | OH2 WAT OH2 WAT | 3500 | -4.211 | 28.797 | 70.359 | 1.00 29.23 |
| MOTA | 20429 | OH2 WAT | | | 28.797 | 70.359 -22.141 | 1.00 29.23 1.00 27.87 |
| ATOM ATOM | 20429 20430 | OH2 WAT OH2 WAT | 3500 | -4.211 | 28.797 | 70.359 | 1.00 29.23 |
| ATOM ATOM ATOM | 20429 20430 20431 | OH2 WAT OH2 WAT OH2 WAT | 3500 3501 | -4.211 23.091 | 28.797 -1.819 | 70.359 -22.141 | 1.00 29.23 1.00 27.87 |

| ATOM | 20434 | OH2 WAT | 3504 | -7.836 | 15.601 | 26.509 | 1.00 22.64 | |
|---|---|---|--|--|--|--|---|-----|
| | | | | | | | | |
| MOTA | 20435 | OH2 WAT | 3505 | | -16.467 | -3.276 | 1.00 30.07 | |
| MOTA | 20436 | OH2 WAT | 3506 | 31.664 | -6.522 | -13.027 | 1.00 22.55 | |
| MOTA | 20437 | OH2 WAT | 3507 | 21.645 | 31.075 | 60.847 | 1.00 17.96 | |
| MOTA | 20438 | OH2 WAT | 3508 | 14.391 | 8.824 | 50.006 | 1.00 23.64 | |
| | 20439 | OH2 WAT | 3509 | -17.132 | 4.640 | 49.766 | 1.00 23.89 | |
| MOTA | | | | | | | | |
| MOTA | 20440 | OH2 WAT | 3510 | | -26.464 | 52.738 | 1.00 30.15 | |
| MOTA | 20441 | OH2 WAT | 3511 | 5.200 | 26.208 | 12.471 | 1.00 34.21 | |
| ATOM | 20442 | OH2 WAT | 3512 | 16.071 | | -25.723 | 1.00 33.79 | |
| | | | | | | | | |
| MOTA | 20443 | OH2 WAT | 3513 | 32.797 | -0.260 | 48.448 | 1.00 20.41 | |
| MOTA | 20444 | OH2 WAT | 3514 | -16.216 | 1.768 | 0.259 | 1.00 23.90 | |
| MOTA | 20445 | OH2 WAT | 3515 | -5.097 | 2.007 | 1.772 | 1.00 19.02 | |
| MOTA | 20446 | OH2 WAT | 3516 | -14.399 | -28.368 | 53.744 | 1.00 43.61 | |
| | | OH2 WAT | 3517 | | -15.041 | 9.961 | 1.00 24.99 | |
| MOTA | 20447 | | | | | | | |
| MOTA | 20448 | OH2 WAT | 3518 | 29.943 | 12.201 | 27.604 | 1.00 32.31 | |
| MOTA | 20449 | OH2 WAT | 3519 | 20.357 | 22.467 | 26.147 | 1.00 24.34 | |
| MOTA | 20450 | OH2 WAT | 3520 | 11.136 | -14.234 | 75.415 | 1.00 25.64 | |
| ATOM | 20451 | OH2 WAT | 3521 | | -15.356 | 56.012 | 1.00 22.35 | |
| | | | | | | | | |
| | 20452 | OH2 WAT | 3522 | | -24.017 | 2.168 | 1.00 29.47 | |
| MOTA | 20453 | OH2 WAT | 3523 | 36.842 | 8.360 | 26.719 | 1.00 24.17 | |
| MOTA | 20454 | OH2 WAT | 3524 | -30.258 | -8.726 | 23.554 | 1.00 27.51 | |
| ATOM | 20455 | OH2 WAT | 3525 | 17.453 | -26.604 | 11.072 | 1.00 24.69 | |
| ATOM | 20456 | OH2 WAT | 3526 | | -51.986 | 25.853 | 1.00 26.03 | |
| | | | | | | | | |
| MOTA | 20457 | OH2 WAT | 3527 | | -21.976 | 39.845 | 1.00 29.39 | |
| MOTA | 20458 | OH2 WAT | 3528 | 29.511 | -4.884 | 16.485 | 1.00 27.39 | |
| MOTA | 20459 | OH2 WAT | 3529 | 14.158 | -1.502 | 9.556 | 1.00 35.97 | |
| ATOM | 20460 | OH2 WAT | 3530 | -14.703 | 20.404 | 38.717 | 1.00 28.71 | |
| | | | | | | | | |
| ATOM | | OH2 WAT | - | -7.105 | | 13.754 | 1.00 18.83 | * * |
| MOTA | 20462 | OH2 WAT | 3532 | 21.848 | -21.505 | 48.844 | 1.00 27.48 | |
| ATOM | 20463 | OH2 WAT | 3533 | 36.224 | -2.915 | 32.963 | 1.00 27.24 | |
| ATOM | 20464 | OH2 WAT | 3534 | 23.251 | 23.615 | 68.702 | 1.00 18.75 | |
| | | OH2 WAT | | -13.136 | | 8.140 | 1.00 22.80 | |
| MOTA | 20465 | | 3535 | | | | | |
| MOTA | 20466 | OH2 WAT | 3536 | -3.662 | 29.839 | 18.235 | 1.00 22.35 | |
| ATOM | 20467 | OH2 WAT | 3537 | 42.444 | -25.120 | 50.779 | 1.00 30.29 | |
| MOTA | 20468 | OH2 WAT | 3538 | 30.684 | 13.800 | 60.308 | 1.00 26.04 | |
| ATOM | 20469 | OH2 WAT | 3539 | -1.141 | 19.587 | 14.828 | 1.00 19.25 | |
| | | | | | | | 1.00 31.13 | |
| ATOM | 20470 | OH2 WAT | 3540 | | -28.227 | 31.527 | | |
| MOTA | 20471 | OH2 WAT | 3541 | 37.483 | -2.016 | 49.590 | 1.00 23.36 | |
| MOTA | 20472 | OH2 WAT | 3542 | -4.059 | -1.055 | -0.721 | 1.00 31.71 | |
| ATOM | 20473 | OH2 WAT | 3543 | 43.257 | -3.965 | 48.382 | 1.00 24.84 | |
| ATOM | | OH2 WAT | 3544 | 16.003 | 15.425 | 17.335 | 1.00 27.51 | |
| | 20474 | | | | | | | |
| MOTA | 20475 | OH2 WAT | 3545 | -12.199 | 21.137 | 35.789 | 1.00 24.22 | |
| MOTA | 20476 | OH2 WAT | 3546 | 43.270 | 11.938 | 40.176 | 1.00 30.17 | |
| MOTA | 20477 | OH2 WAT | 3547 | 8.127 | -56.905 | 24.805 | 1.00 19.10 | |
| MOTA | 20478 | OH2 WAT | 3548 | 20.613 | 33.154 | 62.310 | 1.00 30.19 | |
| | 20479 | OH2 WAT | 3549 | 25.111 | 15.458 | 30.152 | 1.00 22.79 | |
| MOTA | | | | | | | | |
| MOTA | 20480 | OH2 WAT | 3550 | 45.070 | 2.400 | 26.630 | 1.00 30.97 | |
| ATOM | 20481 | OH2 WAT | 3551 | 2.048 | -27.128 | 63.747 | 1.00 22.51 | |
| MOTA | 20482 | 0110 F13 F | 3552 | | 1 632 | | | |
| ATOM | 20483 | OH2 WAT | 222 | -5.000 | 1.032 | -22.794 | 1.00 28.73 | |
| ATOM | | | | | | | | |
| AIOM | | OH2 WAT | 3553 | 40.494 | -30.756 | 61.314 | 1.00 31.19 | |
| 3 55 65 6 | 20484 | OH2 WAT OH2 WAT | 3553 3554 | 40.494 21.635 | -30.756 29.643 | 61.314 51.600 | 1.00 31.19 1.00 24.47 | |
| MOTA | 20484 20485 | OH2 WAT OH2 WAT OH2 WAT | 3553 3554 3555 | 40.494 21.635 20.234 | -30.756 29.643 18.268 | 61.314 51.600 52.367 | 1.00 31.19 1.00 24.47 1.00 25.61 | |
| ATOM ATOM | 20484 | OH2 WAT OH2 WAT | 3553 3554 3555 3556 | 40.494 21.635 20.234 6.420 | -30.756 29.643 18.268 8.840 | 61.314 51.600 52.367 15.848 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 | |
| | 20484 20485 | OH2 WAT OH2 WAT OH2 WAT | 3553 3554 3555 | 40.494 21.635 20.234 | -30.756 29.643 18.268 8.840 | 61.314 51.600 52.367 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 | |
| ATOM ATOM | 20484 20485 20486 20487 | OH2 WAT OH2 WAT OH2 WAT OH2 WAT | 3553 3554 3555 3556 | 40.494 21.635 20.234 6.420 -23.960 | -30.756 29.643 18.268 8.840 | 61.314 51.600 52.367 15.848 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 | |
| ATOM ATOM ATOM | 20484 20485 20486 20487 20488 | OH2 WAT OH2 WAT OH2 WAT OH2 WAT OH2 WAT OH2 WAT | 3553 3554 3555 3556 3557 3558 | 40.494 21.635 20.234 6.420 -23.960 3.694 | -30.756 29.643 18.268 8.840 -31.184 -28.168 | 61.314 51.600 52.367 15.848 20.786 52.744 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 28.76 | |
| ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20489 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 28.76 1.00 29.63 | · |
| ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20489 20490 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 28.76 1.00 29.63 1.00 30.16 | |
| MOTA MOTA MOTA MOTA MOTA MOTA MOTA | 20484 20485 20486 20487 20488 20489 20490 20491 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 28.76 1.00 29.63 1.00 30.16 | · |
| ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20489 20490 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 3562 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 23.44 1.00 30.71 | |
| MOTA MOTA MOTA MOTA MOTA MOTA MOTA | 20484 20485 20486 20487 20488 20489 20490 20491 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 28.76 1.00 29.63 1.00 30.16 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20489 20490 20491 20492 20493 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 3562 3563 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 9.517 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 28.76 1.00 29.63 1.00 30.16 1.00 23.44 1.00 30.71 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20489 20490 20491 20492 20493 20494 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 3562 3563 3564 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 9.517 -16.807 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 23.44 1.00 30.98 1.00 30.98 | |
| MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA | 20484 20485 20486 20487 20488 20489 20490 20491 20492 20493 20494 20495 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 3562 3563 3564 3565 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 9.517 -16.807 14.511 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 23.44 1.00 30.71 1.00 30.98 1.00 33.98 | · |
| MOTA ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20489 20490 20491 20492 20493 20494 20495 20496 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3560 3561 3562 3563 3564 3565 3566 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 1.9517 -16.807 14.511 24.543 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 28.76 1.00 29.63 1.00 30.16 1.00 23.44 1.00 30.71 1.00 30.98 1.00 23.60 1.00 32.53 1.00 27.87 | |
| MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA | 20484 20485 20486 20487 20488 20489 20490 20491 20492 20493 20494 20495 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3560 3561 3562 3563 3564 3565 3566 3567 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 2.422 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 9.517 -16.807 14.511 24.543 29.279 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 73.739 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 33.44 1.00 30.71 1.00 30.98 1.00 23.63 1.00 32.53 1.00 27.87 1.00 26.24 | |
| MOTA ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20489 20490 20491 20492 20493 20494 20495 20496 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3560 3561 3562 3563 3564 3565 3566 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 1.9517 -16.807 14.511 24.543 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 28.76 1.00 29.63 1.00 30.16 1.00 23.44 1.00 30.71 1.00 30.98 1.00 23.60 1.00 32.53 1.00 27.87 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20489 20490 20491 20492 20493 20494 20495 20496 20497 20498 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3560 3561 3562 3563 3564 3564 3565 3566 3567 3568 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 2.422 24.933 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 9.517 -16.807 14.511 24.543 29.279 2.790 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 73.739 38.157 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 30.71 1.00 30.98 1.00 23.60 1.00 32.53 1.00 27.87 1.00 26.24 1.00 31.71 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20489 20490 20491 20492 20493 20494 20495 20496 20497 20498 20499 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 3562 3563 3564 3565 3566 3567 3568 3569 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 2.422 24.933 -6.126 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 9.517 -16.807 14.511 24.543 29.279 31.127 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 73.739 38.157 44.730 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 30.71 1.00 30.98 1.00 32.60 1.00 32.53 1.00 27.87 1.00 26.24 1.00 31.71 1.00 31.71 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20490 20491 20492 20493 20494 20495 20496 20497 20498 20499 20500 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 3562 3563 3564 3565 3566 3567 3568 3569 3570 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 2.422 24.933 -6.126 12.732 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 9.517 -16.807 14.511 24.543 29.279 2.790 31.127 -49.375 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 73.739 38.157 44.730 29.754 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 30.71 1.00 30.98 1.00 32.53 1.00 27.87 1.00 26.24 1.00 24.66 1.00 24.42 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20490 20491 20492 20493 20494 20495 20496 20497 20498 20499 20500 20501 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 3562 3563 3564 3565 3566 3567 3568 3568 3567 3570 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 2.422 24.933 -6.126 12.732 54.364 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 9.517 -16.807 14.511 24.543 29.279 2.790 31.127 -49.375 -4.263 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 73.739 38.157 44.730 29.754 57.668 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 33.44 1.00 30.71 1.00 33.98 1.00 23.60 1.00 23.60 1.00 25.31 1.00 26.24 1.00 24.46 1.00 24.42 1.00 28.75 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20490 20491 20492 20493 20494 20495 20496 20497 20498 20499 20500 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 3562 3563 3564 3565 3566 3567 3568 3569 3570 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 2.422 24.933 -6.126 12.732 54.364 8.524 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 -1.986 32.751 -16.807 14.511 24.543 29.279 2.790 31.127 -49.375 -4.263 5.432 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 73.739 38.157 44.730 29.754 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 30.71 1.00 30.98 1.00 32.53 1.00 27.87 1.00 26.24 1.00 24.66 1.00 24.42 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20490 20491 20492 20493 20495 20496 20497 20498 20499 20500 20501 20502 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 3562 3563 3564 3565 3566 3567 3568 3569 3571 3572 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 2.422 24.933 -6.126 12.732 54.364 8.524 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 -1.986 32.751 -16.807 14.511 24.543 29.279 2.790 31.127 -49.375 -4.263 5.432 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 73.739 38.157 44.730 29.754 57.668 51.993 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 28.76 1.00 29.63 1.00 30.16 1.00 30.71 1.00 30.98 1.00 32.53 1.00 23.60 1.00 23.60 1.00 24.42 1.00 24.42 1.00 28.75 1.00 29.48 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20489 20490 20491 20492 20493 20494 20495 20496 20497 20498 20499 20500 20501 20502 20503 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3560 3561 3562 3563 3564 3565 3566 3567 3568 3569 3570 3571 3572 3573 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 2.422 24.933 -6.126 12.732 54.364 8.524 2.845 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 9.517 -16.807 14.511 24.543 29.279 2.790 31.127 -49.375 -4.263 5.432 -17.320 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 73.739 38.157 44.730 29.754 57.668 51.993 27.601 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 23.44 1.00 30.71 1.00 30.98 1.00 23.60 1.00 32.53 1.00 27.87 1.00 26.24 1.00 31.71 1.00 24.66 1.00 24.42 1.00 28.75 1.00 29.48 1.00 29.48 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20490 20491 20493 20493 20494 20495 20496 20497 20498 20499 20500 20501 20501 20502 20503 20504 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 3562 3563 3564 3565 3566 3567 3570 3571 3572 3573 3574 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 2.422 24.933 -6.126 12.732 54.364 8.524 2.845 -16.502 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 9.517 -16.807 14.511 24.543 29.279 2.790 31.127 -49.375 -4.263 5.432 -17.320 21.486 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 73.739 38.157 44.730 29.754 57.668 57.668 19.93 27.601 18.054 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 33.71 1.00 30.98 1.00 32.53 1.00 23.60 1.00 32.53 1.00 24.66 1.00 24.42 1.00 28.75 1.00 29.48 1.00 29.48 1.00 23.99 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20499 20490 20491 20492 20493 20494 20495 20496 20497 20498 20500 20501 20502 20503 20504 20505 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 3563 3564 3565 3566 3567 3570 3571 3572 3573 3574 3574 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 2.422 24.933 -6.126 12.732 54.364 8.524 2.845 -16.502 43.324 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 9.517 -16.807 14.511 24.543 29.279 31.127 -49.375 -4.263 5.432 -17.320 21.486 21.268 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 73.739 38.157 44.730 29.754 57.668 51.993 27.601 -18.054 62.048 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 30.71 1.00 30.98 1.00 32.53 1.00 27.87 1.00 26.24 1.00 31.71 1.00 24.66 1.00 24.42 1.00 28.75 1.00 29.48 1.00 23.94 1.00 23.94 1.00 23.94 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20490 20491 20493 20493 20494 20495 20496 20497 20498 20499 20500 20501 20501 20502 20503 20504 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 3563 3564 3565 3566 3567 3568 3570 3571 3572 3573 3573 3575 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 2.422 24.933 -6.126 12.732 54.364 8.524 2.845 -16.502 43.324 -13.809 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 9.517 -16.807 14.511 24.543 29.279 2.790 31.127 -49.375 -4.263 5.432 -17.320 21.486 21.268 -17.874 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 73.739 38.157 44.730 29.754 57.668 51.993 27.601 -18.054 62.048 23.626 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 30.71 1.00 33.44 1.00 30.73 1.00 23.60 1.00 32.53 1.00 27.87 1.00 26.24 1.00 31.71 1.00 24.66 1.00 24.42 1.00 28.75 1.00 29.48 1.00 23.94 1.00 23.94 1.00 27.10 1.00 21.29 1.00 21.29 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20499 20490 20491 20492 20493 20494 20495 20496 20497 20498 20500 20501 20502 20503 20504 20505 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 3563 3564 3565 3566 3567 3570 3571 3572 3573 3574 3574 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 2.422 24.933 -6.126 12.732 54.364 8.524 2.845 -16.502 43.324 -13.809 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 9.517 -16.807 14.511 24.543 29.279 31.127 -49.375 -4.263 5.432 -17.320 21.486 21.268 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 73.739 38.157 44.730 29.754 57.668 51.993 27.601 -18.054 62.048 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 30.71 1.00 30.98 1.00 32.53 1.00 27.87 1.00 26.24 1.00 31.71 1.00 24.66 1.00 24.42 1.00 28.75 1.00 29.48 1.00 23.94 1.00 23.94 1.00 23.94 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20490 20491 20492 20494 20495 20496 20497 20500 20501 20502 20503 20505 20506 20507 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 3563 3564 3565 3566 3567 3568 3570 3571 3572 3573 3573 3575 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 2.422 24.933 -6.126 12.732 54.364 8.524 2.845 -16.502 43.324 -13.809 6.416 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 9.517 -16.807 14.511 24.543 29.279 2.790 31.127 -49.375 -4.263 5.432 -17.320 21.486 21.268 -17.874 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 73.739 38.157 44.730 29.754 57.668 51.993 27.601 -18.054 62.048 23.626 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 30.71 1.00 33.44 1.00 30.73 1.00 23.60 1.00 32.53 1.00 27.87 1.00 26.24 1.00 31.71 1.00 24.66 1.00 24.42 1.00 28.75 1.00 29.48 1.00 23.94 1.00 23.94 1.00 27.10 1.00 21.29 1.00 21.29 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20490 20491 20492 20493 20496 20497 20498 20499 20500 20501 20502 20503 20504 20505 20506 20507 20508 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 3562 3563 3564 3565 3566 3567 3570 3571 3572 3573 3574 3575 3576 3576 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 2.422 24.933 -6.126 12.732 54.364 8.524 2.845 -16.502 43.324 -13.809 6.416 23.420 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 9.517 -16.807 14.511 24.543 29.279 2.790 31.127 -49.375 -4.263 5.432 -17.320 21.486 21.268 -17.874 -10.418 -23.177 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 73.739 38.157 44.730 29.754 57.668 51.993 27.601 -18.054 62.048 62.048 63.626 67.564 10.075 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 32.44 1.00 30.71 1.00 32.53 1.00 23.69 1.00 23.60 1.00 24.42 1.00 24.42 1.00 28.75 1.00 29.48 1.00 23.94 1.00 23.94 1.00 23.94 1.00 21.22 1.00 21.22 1.00 25.45 1.00 31.50 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20489 20490 20491 20492 20493 20496 20497 20498 20499 20500 20501 20502 20503 20504 20505 20506 20506 20507 20508 20509 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3560 3561 3562 3563 3564 3565 3566 3567 3572 3573 3574 3575 3577 3578 3577 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 2.422 24.933 -6.126 12.732 54.364 8.524 2.845 -16.502 43.324 -13.809 6.416 23.420 18.146 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 807 14.511 24.543 29.279 2.790 31.127 -49.375 -4.263 5.432 -17.320 21.486 21.268 -17.874 -10.418 -23.177 5.699 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 73.739 38.157 44.730 29.754 57.668 51.993 27.601 -18.054 62.048 23.626 67.564 10.075 42.569 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 23.44 1.00 30.71 1.00 32.53 1.00 23.60 1.00 23.60 1.00 23.60 1.00 24.42 1.00 24.42 1.00 28.75 1.00 24.42 1.00 29.48 1.00 23.94 1.00 21.29 1.00 21.29 1.00 25.45 1.00 25.45 1.00 25.45 | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20484 20485 20486 20487 20488 20490 20491 20492 20493 20496 20497 20498 20499 20500 20501 20502 20503 20504 20505 20506 20507 20508 | OH2 WAT | 3553 3554 3555 3556 3557 3558 3559 3560 3561 3562 3563 3564 3565 3566 3567 3570 3571 3572 3573 3574 3575 3576 3576 | 40.494 21.635 20.234 6.420 -23.960 3.694 -0.279 -13.233 -11.730 25.841 -19.840 35.901 5.279 -12.669 2.422 24.933 -6.126 12.732 54.364 8.524 2.845 -16.502 43.324 -13.809 6.416 23.420 | -30.756 29.643 18.268 8.840 -31.184 -28.168 24.388 -14.029 2.751 -1.986 9.517 -16.807 14.511 24.543 29.279 2.790 31.127 -49.375 -4.263 5.432 -17.320 21.486 21.268 -17.874 -10.418 -23.177 | 61.314 51.600 52.367 15.848 20.786 52.744 69.202 5.054 48.422 41.378 11.289 38.350 23.101 21.588 73.739 38.157 44.730 29.754 57.668 51.993 27.601 -18.054 62.048 62.048 63.626 67.564 10.075 | 1.00 31.19 1.00 24.47 1.00 25.61 1.00 17.10 1.00 23.74 1.00 29.63 1.00 30.16 1.00 32.44 1.00 30.71 1.00 32.53 1.00 23.69 1.00 23.60 1.00 24.42 1.00 24.42 1.00 28.75 1.00 29.48 1.00 23.94 1.00 23.94 1.00 23.94 1.00 21.22 1.00 21.22 1.00 25.45 1.00 31.50 | |

| ATOM | 20511 | OH2 WAT | 3581 | 0.784 -6.629 | 15.625 | 1.00 15.08 |
|------|-------|----------|------|----------------|---------|------------|
| ATOM | 20512 | OH2 WAT | 3582 | 5.497 -17.436 | 23.138 | 1.00 25.09 |
| ATOM | 20513 | OH2 WAT | 3583 | 7.991 6.07 | | 1.00 15.60 |
| ATOM | 20514 | OH2 WAT | 3584 | 3.189 -11.87 | | 1.00 16.47 |
| | | | | -0.207 -12.212 | | 1.00 17.46 |
| MOTA | 20515 | OH2 WAT | 3585 | | | |
| ATOM | 20516 | OH2 WAT | 3586 | 13.002 -15.56 | | 1.00 21.13 |
| MOTA | 20517 | OH2 WAT | 3587 | 20.589 15.73 | | 1.00 26.75 |
| MOTA | 20518 | OH2 WAT | 3588 | 21.090 3.770 | 13.740 | 1.00 22.84 |
| MOTA | 20519 | OH2 WAT | 3589 | 9.607 17.57 | 31.827 | 1.00 19.08 |
| MOTA | 20520 | OH2 WAT | 3590 | 0.276 -14.520 | 35.798 | 1.00 20.57 |
| ATOM | 20521 | OH2 WAT | 3591 | -13.859 19.020 | | 1.00 20.14 |
| ATOM | 20522 | OH2 WAT | 3592 | 22.420 11.92 | | 1.00 18.41 |
| | | | | -3.566 -2.52 | | 1.00 34.12 |
| MOTA | 20523 | OH2 WAT | 3593 | | | |
| MOTA | 20524 | OH2 WAT | 3594 | 24.320 2.280 | | 1.00 24.09 |
| MOTA | 20525 | OH2 WAT | 3595 | 19.088 0.614 | | 1.00 22.35 |
| MOTA | 20526 | OH2 WAT | 3596 | 15.248 1.17 | -17.886 | 1.00 22.97 |
| MOTA | 20527 | OH2 WAT | 3597 | 24.372 9.943 | 24.127 | 1.00 21.06 |
| MOTA | 20528 | OH2 WAT | 3598 | 16.764 -1.79 | 47.475 | 1.00 21.98 |
| ATOM | 20529 | OH2 WAT | 3599 | 0.414 -0.352 | | 1.00 18.76 |
| MOTA | 20530 | OH2 WAT | 3600 | -4.201 -10.540 | | 1.00 23.37 |
| | | OH2 WAT | 3601 | 6.884 -2.27 | | 1.00 28.10 |
| MOTA | 20531 | | | | | |
| MOTA | 20532 | OH2 WAT | 3602 | 23.685 15.179 | | 1.00 22.99 |
| MOTA | 20533 | OH2 WAT | 3603 | 2.551 -10.373 | | 1.00 21.06 |
| ATOM | 20534 | OH2 WAT | 3604 | 21.695 8.786 | 16.503 | 1.00 23.43 |
| MOTA | 20535 | OH2 WAT | 3605 | 12.902 6.15 | 48.325 | 1.00 21.73 |
| ATOM | 20536 | OH2 WAT | 3606 | 9.189 5.244 | 48.426 | 1.00 21.63 |
| ATOM | 20537 | о́н2 waт | 3607 | 2.378 -10.193 | | 1.00 16.25 |
| ATOM | 20538 | OH2 WAT | 3608 | 4.820 -14.21 | | 1.00 30.32 |
| | | OH2 WAT | 3609 | 42.612 26.59 | | 1.00 33.56 |
| ATOM | 20539 | | | | | |
| MOTA | 20540 | OH2 WAT | 3610 | 12.232 -7.07 | | 1.00 15.58 |
| MOTA | 20541 | он2 жат | 3611 | 11.183 -17.229 | | 1.00 22.33 |
| ATOM | 20542 | OH2 WAT | 3612 | 34.209 -6.592 | | 1.00 24.62 |
| ATOM | 20543 | OH2 WAT | 3613 | 6.463 24.23 | 7.734 | 1.00 20.77 |
| ATOM | 20544 | OH2 WAT | 3614 | 33.223 -2.000 | | 1.00 23.63 |
| ATOM | 20545 | OH2 WAT | 3615 | -11.992 -21.34 | | 1.00 21.59 |
| ATOM | 20546 | OH2 WAT | 3616 | 20.404 -27.60 | | 1.00 21.88 |
| | 20547 | OH2 WAT | 3617 | 10.020 -10.31 | | 1.00 30.16 |
| ATOM | | | | | | |
| MOTA | 20548 | OH2 WAT | 3618 | 10.356 -15.159 | | 1.00 21.94 |
| ATOM | 20549 | OH2 WAT | 3619 | 1.389 -11.01 | | 1.00 20.03 |
| MOTA | 20550 | OH2 WAT | 3620 | 4.363 -14.468 | | 1.00 24.43 |
| MOTA | 20551 | OH2 WAT | 3621 | 27.484 2.76 | 55.962 | 1.00 21.15 |
| MOTA | 20552 | OH2 WAT | 3622 | 24.726 -24.180 | 16.875 | 1.00 24.05 |
| ATOM | 20553 | OH2 WAT | 3623 | 0.014 -20.73 | | 1.00 16.17 |
| ATOM | 20554 | OH2 WAT | 3624 | 2.725 4.72 | | 1.00 26.67 |
| | | OH2 WAT | 3625 | 9.746 -14.61 | | 1.00 21.86 |
| MOTA | 20555 | | | | | 1.00 21.00 |
| MOTA | 20556 | OH2 WAT | 3626 | -4.757 -1.899 | | |
| MOTA | 20557 | OH2 WAT | 3627 | 16.835 4.43 | | 1.00 18.72 |
| MOTA | 20558 | OH2 WAT | 3628 | 12.251 -47.69 | | 1.00 22.73 |
| MOTA | 20559 | OH2 WAT | 3629 | 39.019 -10.30 | 16.860 | 1.00 20.92 |
| MOTA | 20560 | OH2 WAT | 3630 | -15.949 -40.71 | 24.697 | 1.00 22.11 |
| ATOM | 20561 | OH2 WAT | 3631 | 25.811 -15.143 | 32.335 | 1.00 27.41 |
| ATOM | | OH2 WAT | 3632 | 15.761 -3.94 | | 1.00 18.59 |
| ATOM | 20563 | OH2 WAT | 3633 | 31.978 -22.98 | | 1.00 27.31 |
| | | OH2 WAT | 3634 | -26.509 -0.17 | | 1.00 18.54 |
| ATOM | 20564 | | | | | 1.00 16.34 |
| MOTA | 20565 | OH2 WAT | 3635 | -15.520 -42.72 | | |
| ATOM | 20566 | OH2 WAT | 3636 | 12.167 -11.989 | | 1.00 19.28 |
| MOTA | 20567 | OH2 WAT | 3637 | -4.154 -47.99 | | 1.00 35.26 |
| MOTA | 20568 | OH2 WAT | 3638 | -1.615 3.19 | | 1.00 25.77 |
| ATOM | 20569 | OH2 WAT | 3639 | -9.493 -3.893 | | 1.00 28.70 |
| ATOM | 20570 | OH2 WAT | 3640 | 16.898 8.348 | -11.925 | 1.00 34.50 |
| MOTA | 20571 | OH2 WAT | 3641 | 32.002 -14.28 | | 1.00 28.21 |
| ATOM | 20572 | OH2 WAT | 3642 | -2.196 -11.14 | | 1.00 24.46 |
| ATOM | 20573 | OH2 WAT | 3643 | 29.916 22.38 | | 1.00 37.43 |
| | 20574 | OH2 WAT | 3644 | 18.608 21.24 | | 1.00 17.98 |
| ATOM | | OH2 WAT | | | | |
| MOTA | 20575 | | 3645 | 38.976 -31.81 | | 1.00 30.85 |
| ATOM | 20576 | OH2 WAT | 3646 | 20.552 -7.819 | | 1.00 25.27 |
| ATOM | 20577 | OH2 WAT | 3647 | 12.060 9.64 | | 1.00 22.18 |
| ATOM | 20578 | OH2 WAT | 3648 | -31.694 -12.59 | | 1.00 34.99 |
| MOTA | 20579 | OH2 WAT | 3649 | 37.537 -7.54 | 19.487 | 1.00 26.06 |
| ATOM | 20580 | OH2 WAT | 3650 | 0.189 -29.389 | 54.461 | 1.00 23.97 |
| MOTA | 20581 | OH2 WAT | 3651 | -5.852 -18.32 | | 1.00 26.63 |
| ATOM | 20582 | OH2 WAT | 3652 | 14.864 -9.33 | | 1.00 20.83 |
| ATOM | 20583 | OH2 WAT | 3653 | | -18.993 | 1.00 25.64 |
| ATOM | 20584 | OH2 WAT | 3654 | -12.613 2.55 | | 1.00 23.04 |
| | | | | 25.889 -19.10 | | |
| ATOM | 20585 | OH2 WAT | 3655 | | | 1.00 24.77 |
| MOTA | 20586 | OH2 WAT | 3656 | 31.173 -1.98 | | 1.00 24.59 |
| MOTA | 20587 | OH2 WAT | 3657 | 40.085 -39.31 | 22.789 | 1.00 28.48 |
| | | | | | | |

| ATOM | 20588 | OH2 | TAW | 3658 | 3.870 -32.022 | 8.417 | 1.00 26.65 |
|------|--------|-----|----------------------------------|--------------|-------------------------|---------|------------|
| ATOM | 20589 | OH2 | WAT | 3659 | 18.544 -28.551 | 16.087 | 1.00 34.40 |
| ATOM | 20590 | OH2 | | 3660 | -6.861 -27.077 | 47.127 | 1.00 22.70 |
| ATOM | 20591 | OH2 | | 3661 | 13.344 -12.961 | 12.757 | 1.00 21.21 |
| ATOM | 20592 | OH2 | | 3662 | 23.924 13.058 | 30.417 | 1.00 26.23 |
| | | | | | | 27.530 | 1.00 23.58 |
| ATOM | 20593 | OH2 | | 3663 | -16.463 0.666 | | |
| MOTA | 20594 | он2 | | 3664 | 29.982 -28.850 | 48.332 | 1.00 25.57 |
| MOTA | 20595 | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3665 | -17.510 7.033 | 13.800 | 1.00 22.45 |
| ATOM | 20596 | OH2 | TAW | 3666 | 1.881 -15.322 | 29.876 | 1.00 24.08 |
| MOTA | 20597 | OH2 | WAT | 3667 | 6.507 -5.396 | 11.525 | 1.00 29.49 |
| ATOM | 20598 | он2 | WAT | 3668 | 46.905 1.491 | 23.229 | 1.00 29.41 |
| ATOM | 20599 | OH2 | | 3669 | -32.090 -8.170 | 19.323 | 1.00 30.01 |
| | 20600 | OH2 | | 3670 | 22.927 -19.385 | 47.561 | 1.00 22.37 |
| ATOM | | | | 3671 | -22.132 17.236 | 0.786 | 1.00 28.38 |
| ATOM | 20601 | OH2 | | | | | |
| MOTA | 20602 | он2 | | 3672 | 33.600 -44.658 | 11.611 | 1.00 34.36 |
| MOTA | 20603 | он2 | | 3673 | -13.806 7.350 | 36.529 | 1.00 29.31 |
| MOTA | 20604 | OH2 | WAT | 3674 | -27.433 -25.257 | 7.569 | 1.00 36.53 |
| ATOM | 20605 | OH2 | WAT | 3675 | -8.731 - 1.580 | 30.817 | 1.00 29.08 |
| ATOM | 20606 | OH2 | WAT | 3676 | 20.432 -3.056 | 56.541 | 1.00 26.44 |
| ATOM | 20607 | он2 | | 3677 | 3.370 -13.090 | 13.599 | 1.00 17.38 |
| ATOM | 20608 | OH2 | | 3678 | 8.012 -34.825 | 12.677 | 1.00 31.51 |
| | 20609 | OH2 | | 3679 | 1.072 -19.415 | 5.239 | 1.00 20.20 |
| ATOM | | | | | | | |
| ATOM | 20610 | OH2 | | 3680 | 21.321 8.443 | 12.592 | 1.00 22.90 |
| MOTA | 20611 | OH2 | | 3681 | 52.644 0.777 | 61.381 | 1.00 35.77 |
| MOTA | 20612 | OH2 | \mathbf{WAT} | 3682 | -3.097 -41.815 | 7.665 | 1.00 31.57 |
| MOTA | 20613 | OH2 | WAT | 3683 | 20.159 -13.750 | 38.154 | 1.00 29.71 |
| MOTA | 20614 | OH2 | TAW | 3684 | -9.685 15.081 | 52.281 | 1.00 25.91 |
| ATOM | 20615 | OH2 | WAT | 3685 | 28.135 20.650 | 0.860 | 1.00 27.21 |
| ATOM | 20616 | OH2 | | 3686 | 39.001 -41.238 | 18.806 | 1.00 26.62 |
| ATOM | 20617 | OH2 | | 3687 | 40.023 -7.002 | 42.151 | 1.00 26.60 |
| | | | | | | 5.482 | 1.00 22.76 |
| MOTA | 20618 | OH2 | | 3688 | | | |
| MOTA | 20619 | он2 | | 3689 | 31.736 -26.387 | 15.172 | 1.00 27.64 |
| MOTA | 20620 | он2 | | 3690 | 37.471 -8.993 | | 1.00 30.40 |
| ATOM | 20621 | OH2 | WAT | 3691 | 10.812 10.675 | 11.247 | 1.00 23.49 |
| ATOM | 20,622 | OH2 | TAW | 3692 | 36.504 -25.533 | 25.441 | 1.00 23.11 |
| ATOM | 20623 | OH2 | WAT | 3693 | 22.254 -32.457 | 61.678 | 1.00 26.40 |
| ATOM | 20624 | OH2 | WAT | 3694 | 11.931 -14.704 | 7.800 | 1.00 21.35 |
| MOTA | 20625 | он2 | | 3695 | -23.681 -14.788 | 45.643 | 1.00 24.78 |
| ATOM | 20626 | OH2 | | 3696 | 7.182 -51.466 | 28.627 | 1.00 25.44 |
| | | OH2 | | 3697 | -22.958 -2.211 | 23.235 | 1.00 26.83 |
| ATOM | 20627 | | | | | | |
| MOTA | 20628 | OH2 | | 3698 | 32.975 -23.395 | -0.121 | 1.00 22.51 |
| MOTA | 20629 | OH2 | | 3699 | -4.858 3.626 | 3.892 | 1.00 28.24 |
| MOTA | 20630 | OH2 | | 3700 | -25.802 - 17.472 | 57.336 | 1.00 24.02 |
| MOTA | 20631 | OH2 | WAT | 3701 | -24.961 -8.029 | 27.571 | 1.00 30.46 |
| ATOM | 20632 | OH2 | WAT | 3702 | -19.843 6.476 | 47.329 | 1.00 25.78 |
| MOTA | 20633 | OH2 | WAT | 3703 | -22.522 14.871 | 2.427 | 1.00 24.66 |
| MOTA | 20634 | | WAT | 3704 | 18.502 41.801 | 32.590 | 1.00 31.05 |
| ATOM | 20635 | | WAT | 3705 | -2.285 23.880 | | 1.00 41.88 |
| | 20636 | | WAT | 3706 | 9.076 7.121 | 12.265 | 1.00 24.55 |
| MOTA | | | | | | | 1.00 24.33 |
| MOTA | 20637 | | WAT | 3707 | 22.472 16.738 | 36.131 | |
| MOTA | 20638 | OH2 | | 3708 | 23.106 19.524 | 28.362 | 1.00 29.35 |
| MOTA | 20639 | OH2 | | 3709 | 20.660 -1.685 | 53.178 | 1.00 28.07 |
| MOTA | 20640 | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3710 | 47.414 -15.667 | 4.341 | 1.00 26.85 |
| MOTA | 20641 | OH2 | \mathbf{WAT} | 3711 | 35.787 -27.874 | 44.447 | 1.00 27.28 |
| MOTA | 20642 | OH2 | \mathbf{WAT} | 3712 | -9.662 17.345 | 32.733 | 1.00 23.43 |
| ATOM | 20643 | OH2 | WAT | 3713 | -23.756 -18.816 | 55.654 | 1.00 27.14 |
| MOTA | 20644 | OH2 | WAT | 3714 | 26.158 -26.333 | 67.093 | 1.00 25.71 |
| ATOM | 20645 | | WAT | 3715 | 8.560 15.732 | 30.041 | 1.00 29.85 |
| MOTA | 20646 | OH2 | | 3716 | 47.272 25.719 | 59.342 | 1.00 32.35 |
| | | OH2 | | | 17.487 -9.851 | -23.543 | 1.00 38.83 |
| MOTA | 20647 | | | 3717 3718 | | 11.110 | 1.00 38.83 |
| ATOM | 20648 | | WAT | | -18.150 -9.422 | | |
| MOTA | 20649 | | TAW | 3719 | 28.787 -33.914 | 15.756 | 1.00 21.48 |
| MOTA | 20650 | | WAT | 3720 | -2.825 9.854 | 58.691 | 1.00 29.62 |
| MOTA | 20651 | OH2 | | 3721 | 35.002 -40.084 | 48.371 | 1.00 34.58 |
| MOTA | 20652 | он2 | WAT | 3722 | 33.278 -36.251 | 12.757 | 1.00 26.17 |
| ATOM | 20653 | он2 | WAT | 3723 | 7.979 -20.213 | 33.159 | 1.00 18.19 |
| MOTA | 20654 | OH2 | WAT | 3724 | -18.398 28.206 | 46.922 | 1.00 33.34 |
| ATOM | 20655 | | WAT | 3725 | 14.111 10.971 | 39.946 | 1.00 39.42 |
| ATOM | 20656 | OH2 | | 3726 | 20.899 -23.856 | 76.684 | 1.00 26.04 |
| ATOM | 20657 | OH2 | | 3727 | 12.600 -30.532 | 39.040 | 1.00 20.04 |
| | | | | | | | |
| ATOM | 20658 | | TAW | 3728 | 0.214 -28.712 | 62.508 | 1.00 28.93 |
| ATOM | 20659 | OH2 | | 3729 | 29.212 -6.590 | 4.979 | 1.00 24.84 |
| MOTA | 20660 | | WAT | 3730 | -17.997 34.615 | 48.280 | 1.00 28.78 |
| MOTA | 20661 | | WAT | 3731 | 21.283 23.102 | 66.907 | 1.00 26.75 |
| MOTA | 20662 | OH2 | TAW | 3732 | 6.942 -10.436 | 70.783 | 1.00 30.98 |
| MOTA | 20663 | OH2 | WAT | 3733 | -13.774 4.431 | 49.066 | 1.00 24.84 |
| MOTA | 20664 | OH2 | WAT | 3734 | 27.594 0.198 | 38.138 | 1.00 33.10 |
| | | | | | | | |

| 3 mos. | 20665 | OTTO WAR | 2725 | 20.794 | 11.104 | 12.321 | 1.00 27.55 |
|--|---|---|--|--|--|--|--|
| MOTA | 20665 | OH2 WAT | 3735 | | | | |
| ATOM | 20666 | OH2 WAT | 3736 | 51.256 | 16.589 | 59.899 | 1.00 30.84 |
| ATOM | 20667 | OH2 WAT | 3737 | 22.183 | -14.735 | 24.243 | 1.00 28.02 |
| | | | | | | | |
| MOTA | 20668 | OH2 WAT | 3738 | 44.096 | -11.703 | 13.054 | 1.00 28.23 |
| ATOM | 20669 | OH2 WAT | 3739 | 18.453 | -23.992 | 49.772 | 1.00 32.67 |
| | | OH2 WAT | 3740 | 10.967 | 16.592 | 34.278 | 1.00 31.80 |
| MOTA | 20670 | | | | | | |
| MOTA | 20671 | OH2 WAT | 3741 | -9.858 | 9.563 | 20.327 | 1.00 20.75 |
| ATOM | 20672 | OH2 WAT | 3742 | 0.898 | 42.404 | 5.444 | 1.00 33.16 |
| | | | | | | | |
| MOTA | 20673 | OH2 WAT | 3743 | 3.933 | -29.127 | 37.039 | 1.00 23.75 |
| ATOM | 20674 | OH2 WAT | 3744 | 36.228 | -24.732 | 33.177 | 1.00 44.37 |
| | | | | | | | 1.00 29.60 |
| ATOM | 20675 | OH2 WAT | 3745 | 3.159 | 7.122 | 37.485 | |
| MOTA | 20676 | OH2 WAT | 3746 | -10.921 | 2.269 | 51.233 | 1.00 27.65 |
| ATOM | 20677 | OH2 WAT | 3747 | 53.348 | 17.944 | 49.378 | 1.00 27.14 |
| | | | | | | | |
| MOTA | 20678 | OH2 WAT | 3748 | 7.606 | 22.178 | 51.653 | 1.00 40.12 |
| ATOM | 20679 | OH2 WAT | 3749 | 39.204 | -34.717 | 27.730 | 1.00 24.03 |
| | 20680 | OH2 WAT | 3750 | 13.564 | 19.874 | 31.976 | 1.00 23.45 |
| MOTA | | | | | | | |
| MOTA | 20681 | OH2 WAT | 3751 | -3.814 | -23.747 | 36.732 | 1.00 26.02 |
| ATOM | 20682 | OH2 WAT | 3752 | 47.146 | 16.831 | 44.337 | 1.00 26.65 |
| | | | | | | | |
| MOTA | 20683 | OH2 WAT | 3753 | | -30.419 | 44.084 | 1.00 25.81 |
| MOTA | 20684 | OH2 WAT | 3754 | 9.861 | -9.263 | 8.727 | 1.00 30.58 |
| ATOM | 20685 | OH2 WAT | 3755 | 23.683 | 32.606 | 59.197 | 1.00 32.94 |
| | | | | | | | |
| MOTA | 20686 | OH2 WAT | 3756 | 20.056 | 31.032 | 18.101 | 1.00 36.08 |
| MOTA | 20687 | OH2 WAT | 3757 | -10.879 | 29.267 | 63.971 | 1.00 35.86 |
| ATOM | 20688 | OH2 WAT | 3758 | | -17.119 | 70.287 | 1.00 32.53 |
| | | | | | | | |
| MOTA | 20689 | OH2 WAT | 3759 | -8.558 | -23.729 | 1.645 | 1.00 40.40 |
| MOTA | 20690 | OH2 WAT | 3760 | -9.873 | 16.727 | 21.573 | 1.00 27.26 |
| | | | | | | | |
| MOTA | 20691 | OH2 WAT | 3761 | | -25.918 | 42.503 | 1.00 30.87 |
| MOTA | 20692 | OH2 WAT | 3762 | 1.971 | 24.125 | 46.097 | 1.00 25.29 |
| MOTA | 20693 | OH2 WAT | 3763 | 53.325 | -5.919 | 60.231 | 1.00 28.08 |
| | | | | | | | |
| MOTA | 20694 | OH2 WAT | 3764 | 10.053 | 18.498 | 6.878 | 1.00 33.94 |
| MOTA | 20695 | OH2 WAT | 3765 | 19.406 | -29.642 | 19.266 | 1.00 28.80 |
| MOTA | 20696 | OH2 WAT | 3766 | 16.098 | 14.581 | 21.816 | 1.00 36.36 |
| | | | | | | * | |
| MOTA | 20697 | OH2 WAT | 3767 | -6.338 | 25.111 | -7.103 | 1.00 28.61 |
| ATOM | 20698 | OH2 WAT | 3768 | 48.102 | 21.342 | 3.587 | 1.00 36.19 |
| | | | | | | | |
| MOTA | 20699 | OH2 WAT | 3769 | | -25.882 | 48.916 | 1.00 39.40 |
| ATOM | 20700 | OH2 WAT | 3770 | 6.373 | 14.161 | 30.878 | 1.00 25.95 |
| ATOM | 20701 | OH2 WAT | 3771 | 18.098 | 37.562 | 30.318 | 1.00 29.01 |
| | | | | | | | |
| MOTA | 20702 | OH2 WAT | 3772 | -4.272 | -41.366 | 30.616 | 1.00 33.77 |
| ATOM | 20703 | OH2 WAT | 3773 | -24.088 | -15.889 | 26.441 | 1.00 33.05 |
| | | | | | | 64.636 | 1.00 43.14 |
| MOTA | 20704 | OH2 WAT | 3774 | 5.765 | 13.265 | | |
| MOTA | 20705 | OH2 WAT | 3775 | -24.832 | -2.210 | 12.951 | 1.00 32.20 |
| MOTA | 20706 | OH2 WAT | 3776 | 35 826 | -23.014 | 22.538 | 1.00 27.58 |
| | | | | | | | |
| MOTA | 20707 | OH2 WAT | 3777 | 34.896 | -31.558 | 17.395 | 1.00 35.22 |
| MOTA | 20708 | OH2 WAT | 3778 | 12.653 | 27.171 | 37.327 | 1.00 34.77 |
| ATOM | 20709 | OH2 WAT | 3779 | 26.085 | 8.717 | 7.225 | 1.00 27.52 |
| | | - | | | | | |
| MOTA | 20710 | OH2 WAT | 3780 | 14.808 | 13.935 | 2.743 | 1.00 28.55 |
| MOTA | 20711 | OH2 WAT | 3781 | 7.008 | 41.307 | 8.799 | 1.00 21.88 |
| | | OH2 WAT | 3782 | | -15.615 | 50.483 | 1.00 33.58 |
| MOTA | 20712 | | | | | | |
| MOTA | 20713 | OH2 WAT | 3783 | 42.042 | 7.501 | 10.339 | 1.00 32.40 |
| ATOM | 20714 | OH2 WAT | 3784 | 38.647 | 27 240 | | |
| | | | | | -37.049 | 26.470 | |
| MOTA | | | | | | 26.470 | 1.00 27.62 |
| | 20715 | OH2 WAT | 3785 | 20.114 | -10.501 | 38.007 | 1.00 27.62 1.00 33.84 |
| MOTA | 20715 | | | | | 38.007 | 1.00 27.62 |
| | 20716 | OH2 WAT OH2 WAT | 3785 3786 | 20.114 33.193 | -10.501 13.567 | 38.007 2.822 | 1.00 27.62 1.00 33.84 1.00 33.07 |
| ATOM | 20716 20717 | OH2 WAT OH2 WAT OH2 WAT | 3785 3786 3787 | 20.114 33.193 41.018 | -10.501 13.567 -5.644 | 38.007 2.822 6.389 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 |
| ATOM ATOM | 20716 20717 20718 | OH2 WAT OH2 WAT OH2 WAT | 3785 3786 3787 3788 | 20.114 33.193 41.018 1.927 | -10.501 13.567 -5.644 13.217 | 38.007 2.822 6.389 17.887 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 |
| ATOM | 20716 20717 | OH2 WAT OH2 WAT OH2 WAT | 3785 3786 3787 | 20.114 33.193 41.018 | -10.501 13.567 -5.644 | 38.007 2.822 6.389 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 |
| MOTA MOTA MOTA | 20716 20717 20718 20719 | OH2 WAT OH2 WAT OH2 WAT OH2 WAT | 3785 3786 3787 3788 3789 | 20.114 33.193 41.018 1.927 0.063 | -10.501 13.567 -5.644 13.217 -39.198 | 38.007 2.822 6.389 17.887 5.123 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 |
| ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 | OH2 WAT OH2 WAT OH2 WAT OH2 WAT OH2 WAT OH2 WAT | 3785 3786 3787 3788 3789 3790 | 20.114 33.193 41.018 1.927 0.063 14.610 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 | 38.007 2.822 6.389 17.887 5.123 49.001 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 23.41 |
| MOTA MOTA MOTA MOTA MOTA MOTA | 20716 20717 20718 20719 20720 20721 | OH2 WAT | 3785 3786 3787 3788 3789 3790 3791 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 23.41 |
| ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 | OH2 WAT OH2 WAT OH2 WAT OH2 WAT OH2 WAT OH2 WAT | 3785 3786 3787 3788 3789 3790 | 20.114 33.193 41.018 1.927 0.063 14.610 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 | 38.007 2.822 6.389 17.887 5.123 49.001 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 23.41 |
| ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 | OH2 WAT | 3785 3786 3787 3788 3789 3790 3791 3792 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 23.41 1.00 29.00 1.00 26.47 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 | OH2 WAT | 3785 3786 3787 3788 3789 3790 3791 3792 3793 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 23.27 1.00 23.25 1.00 40.67 1.00 23.41 1.00 29.00 1.00 26.47 1.00 35.61 |
| ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 | OH2 WAT | 3785 3786 3787 3788 3789 3790 3791 3792 3793 3794 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 -41.765 -48.346 -52.758 19.596 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 23.41 1.00 29.00 1.00 26.47 1.00 35.61 1.00 27.30 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 | OH2 WAT | 3785 3786 3787 3788 3789 3790 3791 3792 3793 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 23.27 1.00 23.25 1.00 40.67 1.00 23.41 1.00 29.00 1.00 26.47 1.00 35.61 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 | OH2 WAT | 3785 3786 3787 3788 3789 3790 3791 3792 3793 3794 3795 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 | 1.00 27.62 1.00 33.84 1.00 32.27 1.00 23.25 1.00 40.67 1.00 23.41 1.00 29.00 1.00 26.47 1.00 35.61 1.00 27.30 1.00 27.60 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 | OH2 WAT | 3785 3786 3787 3788 3789 3790 3791 3792 3793 3794 3795 3796 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 23.41 1.00 29.00 1.00 26.47 1.00 35.61 1.00 27.30 1.00 27.60 1.00 29.51 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 | OH2 WAT | 3785 3786 3787 3788 3789 3790 3791 3792 3793 3794 3795 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 23.41 1.00 29.00 1.00 26.47 1.00 35.61 1.00 27.30 1.00 27.60 1.00 29.51 1.00 26.01 |
| MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 | OH2 WAT | 3785 3786 3787 3788 3789 3790 3791 3792 3793 3794 3795 3796 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 23.41 1.00 29.00 1.00 26.47 1.00 35.61 1.00 27.30 1.00 27.60 1.00 29.51 |
| MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20725 20727 20728 | OH2 WAT | 3785 3786 3787 3788 3790 3791 3792 3793 3794 3795 3796 3797 3798 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 -23.350 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 23.41 1.00 29.00 1.00 26.47 1.00 27.30 1.00 27.60 1.00 29.51 1.00 26.01 1.00 26.06 |
| MOTA ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 20728 20729 | OH2 WAT | 3785 3786 3787 3788 3799 3791 3792 3793 3794 3795 3796 3798 3799 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 -23.350 21.618 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 23.27 1.00 23.25 1.00 40.67 1.00 29.00 1.00 26.47 1.00 27.30 1.00 27.60 1.00 29.51 1.00 26.01 1.00 26.01 1.00 26.06 1.00 30.34 |
| MOTA ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 20728 20729 20730 | OH2 WAT | 3785 3786 3787 3788 3799 3791 3792 3793 3794 3795 3796 3797 3798 3799 3800 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 -23.350 21.618 3.296 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 31.352 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 59.084 | 1.00 27.62 1.00 33.84 1.00 32.27 1.00 32.25 1.00 40.67 1.00 23.41 1.00 29.00 1.00 26.47 1.00 27.30 1.00 27.60 1.00 29.51 1.00 26.06 1.00 26.01 1.00 26.06 1.00 20.90 |
| MOTA ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 20728 20729 20730 | OH2 WAT | 3785 3786 3787 3788 3799 3791 3792 3793 3794 3795 3796 3797 3798 3799 3800 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 -23.350 21.618 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 31.352 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 | 1.00 27.62 1.00 33.84 1.00 32.27 1.00 32.25 1.00 40.67 1.00 23.41 1.00 29.00 1.00 26.47 1.00 27.30 1.00 27.60 1.00 29.51 1.00 26.06 1.00 26.01 1.00 26.06 1.00 20.90 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 20728 20729 20730 20731 | OH2 WAT | 3785 3786 3787 3788 3790 3791 3792 3793 3795 3796 3797 3798 3799 3800 3801 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 -23.350 21.618 3.296 11.215 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 31.352 -4.478 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 59.084 10.504 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 23.41 1.00 25.47 1.00 35.61 1.00 27.30 1.00 27.60 1.00 29.51 1.00 26.01 1.00 26.06 1.00 30.34 1.00 20.90 1.00 20.90 1.00 20.90 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 20728 20729 20730 20731 20732 | OH2 WAT | 3785 3786 3787 3788 3799 3791 3792 3793 3795 3795 3796 3797 3798 3799 3800 3801 3802 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 -23.350 21.618 3.296 11.215 17.465 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 31.352 -4.478 28.856 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 59.084 49.985 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 23.27 1.00 23.25 1.00 40.67 1.00 29.00 1.00 26.47 1.00 27.30 1.00 27.60 1.00 27.60 1.00 26.01 1.00 26.06 1.00 30.34 1.00 20.90 1.00 26.27 1.00 32.00 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 20728 20729 20730 20731 | OH2 WAT | 3785 3786 3787 3788 3790 3791 3792 3793 3795 3796 3797 3798 3799 3800 3801 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 -23.350 21.618 3.296 11.215 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 31.352 -4.478 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 59.084 10.504 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 23.41 1.00 25.47 1.00 35.61 1.00 27.30 1.00 27.60 1.00 29.51 1.00 26.01 1.00 26.06 1.00 30.34 1.00 20.90 1.00 20.90 1.00 20.90 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20725 20726 20727 20728 20729 20730 20731 20732 20733 | OH2 WAT | 3785 3786 3787 3788 3799 3790 3791 3792 3793 3794 3795 3796 3797 3798 3800 3800 3802 3803 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 -23.350 21.618 3.296 11.215 17.465 30.546 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 31.352 -4.478 28.856 21.709 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 59.084 10.504 49.985 36.983 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 23.27 1.00 23.25 1.00 40.67 1.00 29.00 1.00 26.47 1.00 27.30 1.00 27.60 1.00 27.60 1.00 26.01 1.00 26.06 1.00 30.34 1.00 20.27 1.00 26.27 1.00 32.00 1.00 33.86 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 20728 20730 20731 20731 20733 20734 | OH2 WAT | 3785 3786 3787 3788 3799 3791 3792 3793 3794 3795 3797 3798 3799 3800 3801 3802 3803 3804 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.766 34.924 -23.350 21.618 3.296 11.215 17.465 30.546 -13.822 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 31.352 -4.478 28.856 21.709 6.385 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 59.084 10.504 49.985 36.983 18.289 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 29.00 1.00 26.47 1.00 27.30 1.00 27.30 1.00 27.60 1.00 29.51 1.00 26.01 1.00 26.06 1.00 30.34 1.00 20.90 1.00 26.27 1.00 32.00 1.00 33.86 1.00 36.93 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 20728 20729 20730 20731 20732 20733 20734 20735 | OH2 WAT | 3785 3786 3787 3788 3799 3791 3792 3793 3794 3795 3797 3798 3799 3800 3801 3802 3803 3804 3805 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 -23.350 21.618 3.296 11.215 17.465 30.546 -13.822 40.370 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 31.352 -4.478 28.856 21.709 6.385 26.108 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 59.084 10.504 49.985 36.983 18.289 57.308 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 23.27 1.00 23.25 1.00 40.67 1.00 29.00 1.00 26.47 1.00 27.30 1.00 27.60 1.00 29.51 1.00 26.01 1.00 26.06 1.00 30.34 1.00 20.90 1.00 26.27 1.00 32.00 1.00 33.86 1.00 26.93 1.00 33.33 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 20728 20730 20731 20731 20733 20734 | OH2 WAT | 3785 3786 3787 3788 3799 3791 3792 3793 3794 3795 3797 3798 3799 3800 3801 3802 3803 3804 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.766 34.924 -23.350 21.618 3.296 11.215 17.465 30.546 -13.822 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 31.352 -4.478 28.856 21.709 6.385 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 59.084 10.504 49.985 36.983 18.289 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 29.00 1.00 26.47 1.00 27.30 1.00 27.30 1.00 27.60 1.00 29.51 1.00 26.01 1.00 26.06 1.00 30.34 1.00 20.90 1.00 26.27 1.00 32.00 1.00 33.86 1.00 36.93 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 20728 20730 20731 20733 20733 20734 20735 20736 | OH2 WAT | 3785 3786 3787 3788 3799 3791 3792 3793 3794 3795 3796 3799 3800 3801 3802 3803 3804 3805 3806 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 -23.350 21.618 3.296 11.215 17.465 30.546 -13.822 40.370 -18.730 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 31.352 -4.478 28.856 21.709 6.385 26.108 19.657 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 59.084 10.504 49.985 36.983 18.289 57.308 0.767 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 23.41 1.00 25.00 1.00 27.30 1.00 27.30 1.00 27.60 1.00 26.01 1.00 26.01 1.00 26.01 1.00 26.06 1.00 20.90 1.00 30.34 1.00 20.90 1.00 33.86 1.00 30.34 1.00 20.90 1.00 26.27 1.00 32.00 1.00 33.32 1.00 33.23 1.00 33.23 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 20728 20730 20731 20733 20734 20735 20736 20737 | OH2 WAT | 3785 3786 3787 3788 3799 3791 3792 3793 3795 3796 3797 3798 3799 3801 3802 3803 3804 3804 3806 3807 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 -23.350 21.618 3.296 11.215 17.465 30.546 -13.822 40.370 -18.730 46.787 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 31.352 -4.478 28.856 21.709 6.385 26.108 19.657 -11.310 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 59.084 10.504 49.985 36.983 18.289 57.308 0.767 5.258 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 23.41 1.00 25.47 1.00 35.61 1.00 27.30 1.00 27.60 1.00 29.51 1.00 26.01 1.00 26.06 1.00 30.34 1.00 20.90 1.00 30.34 1.00 33.86 1.00 26.93 1.00 33.23 1.00 34.40 1.00 33.73 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 20728 20730 20731 20733 20734 20735 20736 20737 | OH2 WAT | 3785 3786 3787 3788 3799 3791 3792 3793 3795 3796 3797 3798 3799 3800 3801 3802 3803 3804 3805 3806 3807 3808 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 -23.350 21.618 3.296 11.215 17.465 30.546 -13.822 40.370 -18.730 46.787 6.196 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 31.352 -4.478 28.856 21.709 6.385 26.108 19.657 -11.310 37.401 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 59.084 49.985 36.983 18.289 57.308 0.767 5.258 65.886 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 29.00 1.00 26.47 1.00 27.30 1.00 27.60 1.00 27.60 1.00 26.01 1.00 26.01 1.00 20.90 1.00 30.34 1.00 20.90 1.00 33.86 1.00 26.93 1.00 33.23 1.00 34.40 1.00 33.73 1.00 25.32 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 20728 20730 20731 20733 20734 20735 20736 20737 | OH2 WAT | 3785 3786 3787 3788 3799 3791 3792 3793 3795 3796 3797 3798 3799 3801 3802 3803 3804 3804 3806 3807 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 -23.350 21.618 3.296 11.215 17.465 30.546 -13.822 40.370 -18.730 46.787 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 31.352 -4.478 28.856 21.709 6.385 26.108 19.657 -11.310 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 59.084 10.504 49.985 36.983 18.289 57.308 0.767 5.258 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 32.27 1.00 23.25 1.00 40.67 1.00 23.41 1.00 25.47 1.00 35.61 1.00 27.30 1.00 27.60 1.00 29.51 1.00 26.01 1.00 26.06 1.00 30.34 1.00 20.90 1.00 30.34 1.00 33.86 1.00 26.93 1.00 33.23 1.00 34.40 1.00 33.73 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 20730 20731 20732 20733 20734 20735 20736 20737 20738 20738 | OH2 WAT | 3785 3786 3787 3788 3799 3791 3792 3793 3794 3795 3796 3797 3798 3800 3801 3802 3803 3804 3805 3806 3807 3808 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 -23.350 21.618 3.296 11.215 17.465 30.546 -13.822 40.370 -18.730 46.787 6.196 33.898 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 31.352 -4.478 28.856 21.709 6.385 26.108 19.657 -11.310 37.401 -16.337 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 59.084 10.504 49.985 36.983 18.289 57.308 0.767 5.258 65.886 34.979 | 1.00 27.62 1.00 33.84 1.00 33.84 1.00 33.27 1.00 23.25 1.00 40.67 1.00 29.00 1.00 26.47 1.00 27.30 1.00 27.60 1.00 27.60 1.00 26.01 1.00 26.06 1.00 30.34 1.00 20.97 1.00 32.00 1.00 33.86 1.00 26.93 1.00 33.73 1.00 33.73 1.00 35.93 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 20730 20731 20733 20734 20735 20736 20737 20738 20738 20739 20738 | OH2 WAT | 3785 3786 3787 3788 3789 3791 3792 3793 3795 3795 3797 3798 3799 3800 3801 3802 3803 3804 3805 3806 3807 3808 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 -23.350 21.618 3.296 11.215 17.465 30.546 -13.822 40.370 -18.730 46.787 6.196 33.898 -29.017 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 31.352 -4.478 28.856 21.709 6.385 26.108 19.657 -11.310 37.401 -16.337 -32.892 | 38.007 2.822 6.389 17.887 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 59.084 10.504 49.985 36.983 18.289 57.308 0.767 5.258 634.979 18.794 | 1.00 27.62 1.00 33.84 1.00 33.07 1.00 23.27 1.00 23.25 1.00 40.67 1.00 29.00 1.00 26.47 1.00 27.30 1.00 27.30 1.00 27.60 1.00 29.51 1.00 26.06 1.00 30.34 1.00 20.90 1.00 26.27 1.00 32.00 1.00 32.00 1.00 33.86 1.00 33.86 1.00 33.36 1.00 33.37 1.00 34.70 |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 20716 20717 20718 20719 20720 20721 20722 20723 20724 20725 20726 20727 20730 20731 20732 20733 20734 20735 20736 20737 20738 20738 | OH2 WAT | 3785 3786 3787 3788 3799 3791 3792 3793 3794 3795 3796 3797 3798 3800 3801 3802 3803 3804 3805 3806 3807 3808 | 20.114 33.193 41.018 1.927 0.063 14.610 29.017 16.478 2.863 -11.416 32.706 3.656 34.924 -23.350 21.618 3.296 11.215 17.465 30.546 -13.822 40.370 -18.730 46.787 6.196 33.898 | -10.501 13.567 -5.644 13.217 -39.198 -2.645 -41.765 28.346 -52.758 19.596 -47.734 6.892 -21.245 8.284 5.515 31.352 -4.478 28.856 21.709 6.385 26.108 19.657 -11.310 37.401 -16.337 | 38.007 2.822 6.389 17.887 5.123 49.001 34.853 37.634 24.049 17.671 14.100 17.830 -11.957 62.170 19.392 59.084 10.504 49.985 36.983 18.289 57.308 0.767 5.258 65.886 34.979 | 1.00 27.62 1.00 33.84 1.00 33.84 1.00 33.27 1.00 23.25 1.00 40.67 1.00 29.00 1.00 26.47 1.00 27.30 1.00 27.60 1.00 27.60 1.00 26.01 1.00 26.06 1.00 30.34 1.00 20.97 1.00 32.00 1.00 33.86 1.00 26.93 1.00 33.73 1.00 33.73 1.00 35.93 |

| ATOM | 20742 | OH2 | WAT | 3812 | 7.988 | -3.484 | 64.242 | 1.00 31.97 |
|------|--------|-----|----------------------------------|------|---------|---------|---------|------------|
| | | | | 3813 | 5.432 | -9.598 | 10.054 | 1.00 29.06 |
| ATOM | 20743 | | TAW | | - | | | |
| ATOM | 20744 | | TAW | 3814 | 19.243 | 6.256 | -9.064 | 1.00 30.91 |
| MOTA | 20745 | OH2 | TAW | 3815 | 43.635 | -21.259 | 49.737 | 1.00 28.64 |
| ATOM | 20746 | OH2 | WAT | 3816 | -5.313 | 6.920 | 37.151 | 1.00 30.93 |
| ATOM | 20747 | OH2 | WAT | 3817 | 4.504 | 24.582 | -5.136 | 1.00 32.05 |
| ATOM | 20748 | OH2 | WAT | 3818 | 10.520 | 3.740 | -26.086 | 1.00 34.31 |
| ATOM | 20749 | | WAT | 3819 | 62.545 | 14.377 | 25.314 | 1.00 43.40 |
| | | | | | | -15.964 | 13.553 | 1.00 29.65 |
| MOTA | 20750 | | TAW | 3820 | | | | |
| MOTA | 20751 | | WAT | 3821 | | -50.398 | 19.754 | 1.00 33.87 |
| MOTA | 20752 | OH2 | \mathbf{WAT} | 3822 | 2.304 | -6.547 | 19.517 | 1.00 31.26 |
| MOTA | 20753 | OH2 | WAT | 3823 | 41.519 | -23.035 | -7.279 | 1.00 42.38 |
| ATOM | 20754 | OH2 | WAT | 3824 | 16.162 | -20.007 | 75.071 | 1.00 26.45 |
| ATOM | 20755 | OH2 | WAT | 3825 | 10.546 | -21.372 | 6.968 | 1.00 26.45 |
| ATOM | 20756 | | WAT | 3826 | | -23.711 | 34.633 | 1.00 29.90 |
| | | | WAT | 3827 | | -28.322 | 57.340 | 1.00 41.11 |
| MOTA | 20757 | | | | | | | |
| MOTA | 20758 | | TAW | 3828 | | -17.624 | 23.792 | 1.00 26.84 |
| MOTA | 20759 | OH2 | WAT | 3829 | -10.831 | -0.831 | 4.970 | 1.00 24.36 |
| MOTA | 20760 | OH2 | WAT | 3830 | 7.070 | 13.238 | -20.561 | 1.00 30.58 |
| MOTA | 20761 | OH2 | WAT | 3831 | -1.423 | -43.194 | 35.158 | 1.00 28.74 |
| ATOM | 20762 | OH2 | WAT | 3832 | 16.519 | -33.636 | 38.322 | 1.00 24.42 |
| MOTA | 20763 | | WAT | 3833 | 17.520 | 22.887 | 73.186 | 1.00 33.05 |
| | | | | | -2.872 | -6.802 | 25.146 | 1.00 32.72 |
| MOTA | 20764 | | TAW | 3834 | | | | |
| MOTA | 20765 | | WAT | 3835 | | -54.085 | 15.078 | 1.00 34.15 |
| MOTA | 20766 | OH2 | \mathbf{WAT} | 3836 | 41.800 | -20.963 | 55.130 | 1.00 27.59 |
| ATOM | 20767 | OH2 | WAT | 3837 | -7.482 | -4.152 | 30.462 | 1.00 29.41 |
| ATOM | 20768 | OH2 | TAW | 3838 | -17.203 | -14.842 | 28.926 | 1.00 26.31 |
| ATOM | 20769 | | WAT | 3839 | 23.941 | 17.177 | 27.224 | 1.00 23.52 |
| ATOM | 20770 | | WAT | 3840 | -17.547 | | -10.035 | 1.00 26.05 |
| | | | | | | | 19.442 | 1.00 29.94 |
| MOTA | 20771 | | TAW | 3841 | -11.739 | 21.608 | | |
| MOTA | 20772 | | WAT | 3842 | | -31.809 | 56.054 | 1.00 29.15 |
| MOTA | 20773 | OH2 | WAT | 3843 | | -28.472 | 40.778 | 1.00 31.95 |
| MOTA | .20774 | OH2 | WAT | 3844 | 13.649 | -18.971 | 8.359 | 1.00 28.20 |
| ATOM | 20775 | OH2 | WAT | 3845 | -1.364 | 38.574 | 55.862 | 1.00 34.22 |
| MOTA | 20776 | OH2 | WAT | 3846 | 49.423 | 21.080 | 55.366 | 1.00 24.86 |
| MOTA | 20777 | | WAT | 3847 | | -12.614 | 7.599 | 1.00 38.86 |
| | 20778 | | WAT | 3848 | | -53.041 | 14.218 | 1.00 31.46 |
| MOTA | | | | | | | | |
| MOTA | 20779 | | TAW | 3849 | | -31.885 | 21.029 | 1.00 27.96 |
| MOTA | 20780 | | WAT | 3850 | | -35.638 | 34.940 | 1.00 25.32 |
| MOTA | 20781 | OH2 | WAT | 3851 | -0.470 | 22.594 | 36.668 | 1.00 25.41 |
| ATOM | 20782 | OH2 | WAT | 3852 | -1.223 | -1.667 | 38.153 | 1.00 24.06 |
| MOTA | 20783 | OH2 | WAT | 3853 | 24.503 | -1.990 | 58.124 | 1.00 28.69 |
| MOTA | 20784 | | WAT | 3854 | | -13.588 | 29.400 | 1.00 23.88 |
| ATOM | 20785 | | WAT | 3855 | | -14.815 | 57.051 | 1.00 26.82 |
| | | | | | 20.622 | -5.682 | 38.418 | 1.00 20.02 |
| MOTA | 20786 | | | 3856 | | | | |
| MOTA | 20787 | он2 | WAT | 3857 | - | -24.739 | 4.250 | 1.00 36.23 |
| MOTA | 20788 | OH2 | WAT. | 3858 | 50.437 | -6.107 | 52.678 | 1.00 25.23 |
| MOTA | 20789 | OH2 | \mathbf{WAT} | 3859 | -32.230 | -8.257 | 14.449 | 1.00 36.13 |
| MOTA | 20790 | OH2 | WAT | 3860 | 24.061 | -50.798 | 39.085 | 1.00 41.51 |
| ATOM | 20791 | OH2 | WAT | 3861 | 29.292 | 7.952 | 26.061 | 1.00 36.29 |
| MOTA | 20792 | | WAT | 3862 | 37.184 | 10.315 | 28.928 | 1.00 28.67 |
| ATOM | 20793 | | WAT | 3863 | | -20.183 | 38.839 | 1.00 25.50 |
| | 20794 | | WAT | 3864 | -0.607 | 5.406 | 54.644 | 1.00 23.50 |
| MOTA | | | | | | | | |
| MOTA | 20795 | | TAW | 3865 | 11.302 | -47.890 | 27.551 | 1.00 20.57 |
| MOTA | 20796 | | WAT | 3866 | -15.007 | 23.732 | 62.688 | |
| MOTA | 20797 | | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3867 | | -21.336 | 46.400 | 1.00 28.39 |
| MOTA | 20798 | OH2 | WAT | 3868 | 32.816 | 16.299 | 26.091 | 1.00 28.85 |
| MOTA | 20799 | OH2 | WAT | 3869 | 15.315 | 17.295 | 25.040 | 1.00 20.18 |
| MOTA | 20800 | он2 | WAT | 3870 | 7.289 | -17.152 | -3.029 | 1.00 29.44 |
| ATOM | 20801 | | WAT | 3871 | 2.717 | 42.008 | 66.372 | 1.00 27.89 |
| | | | | | 34.914 | -28.691 | 18.175 | 1.00 19.17 |
| MOTA | 20802 | OH2 | WAT | 3872 | | | | |
| ATOM | 20803 | | WAT | 3873 | 18.616 | 13.919 | 13.090 | 1.00 32.78 |
| MOTA | 20804 | он2 | WAT | 3874 | -18.466 | -37.393 | 25.244 | 1.00 32.88 |
| MOTA | 20805 | | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3875 | 12.836 | 43.517 | 24.922 | 1.00 31.86 |
| MOTA | 20806 | он2 | WAT | 3876 | -25.602 | 12.369 | 0.165 | 1.00 27.51 |
| MOTA | 20807 | он2 | WAT | 3877 | 24.200 | 7.550 | 21.778 | 1.00 31.56 |
| ATOM | 20808 | | WAT | 3878 | -0.145 | -8.461 | 22.519 | 1.00 26.05 |
| ATOM | 20809 | | WAT | 3879 | -23.514 | -16.029 | 43.033 | 1.00 33.79 |
| | | | | | | | -0.282 | |
| MOTA | 20810 | | WAT | 3880 | 9.948 | 50.191 | | 1.00 30.98 |
| MOTA | 20811 | | WAT | 3881 | 2.703 | -13.370 | 5.739 | 1.00 35.46 |
| MOTA | 20812 | | TAW | 3882 | 20.914 | 25.963 | 17.772 | 1.00 28.78 |
| MOTA | 20813 | | \mathbf{WAT} | 3883 | 34.528 | 11.261 | 3.220 | 1.00 31.17 |
| ATOM | 20814 | он2 | WAT | 3884 | 16.134 | -53.497 | 28.465 | 1.00 33.54 |
| ATOM | 20815 | он2 | WAT | 3885 | -2.387 | 38.437 | 61.965 | 1.00 31.00 |
| MOTA | 20816 | он2 | | 3886 | 43.549 | -6.595 | 8.700 | 1.00 33.92 |
| ATOM | 20817 | | WAT | 3887 | 35.170 | -2.113 | 5.111 | 1.00 23.74 |
| MOTA | 20818 | | WAT | 3888 | -25.332 | -27.546 | 33.584 | 1.00 23.74 |
| AION | 20010 | UNZ | AALTI | 2000 | -23.332 | 27.540 | 22.204 | 1.00 32.00 |

| ATOM | 20819 | он2 | WAT | 3889 | 9.100 | 5.403 | 58.911 | 1.00 28.07 |
|--------------|----------------|-----|----------------------------------|--------------|-------------------|--------------------|------------------|--------------------------|
| ATOM | 20820 | | WAT | 3890 | -2.005 | 3.998 | 40.706 | 1.00 30.75 |
| ATOM | 20821 | | TAW | 3891 | -7.292 | -27.296 | 1.998 | 1.00 38.01 |
| ATOM | 20822 | OH2 | WAT | 3892 | 19.157 | -5.927 | 15.506 | 1.00 31.49 |
| ATOM | 20823 | он2 | WAT | 3893 | -18.372 | 23.651 | 43.344 | 1.00 37.66 |
| ATOM | 20824 | OH2 | WAT | 3894 | 31.262 | -51.492 | 16.861 | 1.00 24.13 |
| ATOM | 20825 | он2 | WAT | 3895 | -26.499 | 9.900 | 3.726 | 1.00 39.65 |
| ATOM | 20826 | он2 | WAT | 3896 | 4.097 | 31.182 | 75.075 | 1.00 32.65 |
| ATOM | 20827 | он2 | TAW | 3897 | 2.547 | 4.374 | 39.181 | 1.00 30.86 |
| ATOM | 20828 | | WAT | 3898 | 15.775 | -19.780 | -5.586 | 1.00 40.14 |
| ATOM | 20829 | OH2 | WAT | 3899 | 25.581 | -38.670 | 36.519 | 1.00 28.00 |
| MOTA | 20830 | OH2 | WAT | 3900 | -5.538 | -11.112 | 0.952 | 1.00 35.04 |
| ATOM | 20831 | OH2 | WAT | 3901 | 22.835 | -4.612 | 16.494 | 1.00 29.12 |
| ATOM | 20832 | он2 | WAT | .3902 | 12.797 | 17.517 | 28.765 | 1.00 25.18 |
| ATOM | 20833 | OH2 | TAW | 3903 | 4.058 | -26.546 | 4.576 | 1.00 30.15 |
| ATOM | 20834 | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3904 | 29.516 | -1.506 | 18.4 İ 2 | 1.00 35.13 |
| ATOM | 20835 | он2 | WAT | 3905 | 8.641 | -41.868 | 14.364 | 1.00 24.18 |
| MOTA | 20836 | он2 | \mathbf{WAT} | 3906 | 17.066 | 16.097 | 14.366 | 1.00 23.39 |
| MOTA | 20837 | OH2 | WAT | 3907 | 24.988 | -0.851 | -20.057 | 1.00 29.57 |
| MOTA | 20838 | он2 | WAT | 3908 | -5.479 | -33.973 | 28.883 | 1.00 27.02 |
| ATOM | 20839 | OH2 | TAW | 3909 | -35.530 | -14.033 | 12.897 | 1.00 34.50 |
| MOTA | 20840 | он2 | TAW | 3910 | -19.863 | 23.952 | 46.624 | 1.00 32.52 |
| MOTA | 20841 | он2 | WAT | 3911 | 11.250 | -32.899 | 13.772 | 1.00 26.39 |
| MOTA | 20842 | OH2 | TAW | 3912 | 18.533 | 26.176 | 31.373 | 1.00 26.30 |
| MOTA | 20843 | OH2 | WAT | 3913 | 11.461 | -44.385 | 34.329 | 1.00 36.66 |
| MOTA | 20844 | OH2 | WAT | 3914 | 49.046 | 8.099 | 27.030 | 1.00 31.36 |
| ATOM | 20845 | OH2 | TAW | 3915 | -6.962 | 47.797 | 20.546 | 1.00 35.11 |
| ATOM | 20846 | OH2 | TAW | 3916 | -11.454 | 27.697 | 39.038 | 1.00 34.68 |
| MOTA | 20847 | он2 | TAW | 3917 | -17.534 | -6.063 | -15.347 | 1.00 33.23 |
| MOTA | 20848 | OH2 | WAT | 3918 | -20.662 | 24.797 | 51.285 | 1.00 38.11 |
| MOTA | 20849 | OH2 | WAT | 3919 | -15.182 | 22.940 | -8.359 | 1.00 32.06 |
| MOTA | 20850 | OH2 | WAT | 3920 | -5.318 | 20.153 | -21.024 | 1.00 36.60 |
| MOTA | 20851 | OH2 | WAT | 3921 | 29.287 | 32.027 | 23.219 | 1.00 29.21 |
| MOTA | 20852 | OH2 | WAT | 3922 | 5.296 | 4.996 | 60.230 | 1.00 27.47 |
| ATOM | 20853 | OH2 | WAT | 3923 | 0.917 | -45.819 | 34.364 | 1.00 33.20 |
| MOTA | 20854 | OH2 | WAT | 3924 | 3.488 | 6.382 | 55.858 | 1.00 25.52 |
| MOTA | 20855 | он2 | WAT | 3925 | 32.958 | 6.677 | 47.699 | 1.00 22.12 |
| MOTA | 20856 | OH2 | WAT | 3926 | -23.321 | -11.254 | 27.790 | 1.00 35.27 |
| MOTA | 20857 | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3927 | 32.860 | 27.703 | 46.551 | 1.00 32.44 |
| MOTA | 20858 | OH2 | WAT | 3928 | -1.426 | 25.054 | 11.614 | 1.00 29.69 |
| MOTA | 20859 | OH2 | TAW | 3929 | -15.519 | 16.582 | 14.184 | 1.00 28.11 |
| MOTA | 20860 | OH2 | WAT | 3930 | 43.595 | | 8.451 | 1.00 30.25 |
| MOTA | 20861 | | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3931 | 23.063 | 6.691 | 36.902 | 1.00 33.20 |
| MOTA | 20862 | | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3932 | -9.032 | 1.177 | 27.078 | 1.00 34.25 |
| MOTA | 20863 | | WAT | 3933 | 31.257 | 21.599 | 1.621 | 1.00 37.72 |
| MOTA | 20864 | | WAT | 3934 | 38.507 | -21.072 | | 1.00 25.61 |
| MOTA | 20865 | | TAW | 3935. | -23.025 | | -10.126 | 1.00 28.93 |
| MOTA | 20866 | | WAT | 3936 | 22.699 | -11.887 | 36.490 | 1.00 24.74 |
| MOTA | 20867 | | WAT | 3937 | 17.275 | -3.978 | 40.410 | 1.00 32.51 |
| MOTA | 20868 | | WAT | 3938 | 7.861 | | 34.973 | 1.00 44.23 |
| MOTA | 20869 | | WAT | 3939 | 11.275 | 25.692 | 34.511 | 1.00 32.64 |
| ATOM | 20870 | OH2 | | 3940 | | -38.226 | | 1.00 33.46 |
| ATOM | 20871 | | TAW | 3941 | | -42.437 | 29.109 | 1.00 43.80 |
| MOTA | 20872 | | WAT | 3942 | | 31.441 | 25.663 | 1.00 37.38 |
| ATOM | 20873 | | WAT | 3943 | | -21.794 | 42.793 | 1.00 34.53 |
| MOTA | 20874 | | WAT | 3944 | -3.638 | 41.102 | 62.525 | 1.00 37.56 |
| MOTA | 20875 | | WAT | 3945 | -18.227 | 25.816 | 55.937 | 1.00 30.59 |
| ATOM | 20876 | | WAT | 3946 | | -38.554 | 28.518 | 1.00 32.77 |
| MOTA | 20877 | | TAW | 3947 | 34.669 | | 67.209 | 1.00 25.76 |
| MOTA | 20878 | | WAT | 3948 | 54.577 | | 52.543 | 1.00 33.52 |
| ATOM | 20879 | | TAW | 3949 | | -14.120 | 4.073 | 1.00 36.74 |
| MOTA | 20880 | | WAT | 3950 | -15.097 | | 18.039 | 1.00 37.02 |
| ATOM | 20881 | | TAW | 3951 | 15.818 | | 9.301 | 1.00 29.29 |
| MOTA | 20882 | | WAT | 3952 | -22.631 | | -14.709 | 1.00 23.92 |
| ATOM | 20883 | | WAT | 3953 | | -17.635 -11.665 | 32.905 68:949 | 1.00 29.71 1.00 36.66 |
| ATOM | 20884 | | WAT TAW | 3954 | -24.033 31 947 | -26.774 | 44.122 | 1.00 36.66 |
| ATOM | 20885 | | WAT WAT | 3955 | | -26.774 -23.512 | 73.698 | 1.00 27.95 |
| ATOM ATOM | 20886 20887 | | WAT | 3956 3957 | 40.516 | | 40.033 | 1.00 34.23 |
| ATOM | 20887 | | WAT | 3957 | | -38.079 | 25.502 | 1.00 37.10 |
| ATOM | 20889 | | WAT | 3959 | 27.138 | | 22.971 | 1.00 23.71 |
| ATOM | 20890 | | WAT | 3960 | 6.627 | | 67.881 | 1.00 23.72 |
| ATOM | 20891 | | WAT | 3961 | -7.495 | | 65.877 | 1.00 33.43 |
| ATOM | 20892 | | WAT | 3962 | | -16.981 | 59.063 | 1.00 41.80 |
| ATOM | 20893 | | WAT | 3963 | 10.451 | | 11.902 | 1.00 42.44 |
| ATOM | 20894 | | WAT | 3964 | -19.187 | | 7.811 | 1.00 34.07 |
| ATOM | 20895 | | WAT | 3965 | 55.677 | | 57.068 | 1.00 34.33 |
| | | | · · · | | | | | - |

| ATOM | 20896 | он2 | WAT | 3966 | -21.554 | 13.101 | 7.475 | 1.00 24.12 |
|--------------|----------------|-----|----------------------------------|------|---------|---------|---------|------------|
| ATOM | 20897 | | WAT | 3967 | 8.150 | -27.034 | 50.434 | 1.00 39.84 |
| ATOM | 20898 | | WAT | 3968 | -18.831 | 9.121 | 46.959 | 1.00 30.55 |
| | | | | | 50.680 | 1.961 | 15.800 | 1.00 35.02 |
| MOTA | 20899 | | TAW | 3969 | | | | |
| MOTA | 20900 | | TAW | 3970 | 35.217 | | 25.289 | 1.00 34.87 |
| MOTA | 20901 | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3971 | -29.398 | -8.042 | 11.100 | 1.00 31.40 |
| MOTA | 20902 | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3972 | 19.447 | 17.441 | 13.441 | 1.00 29.33 |
| ATOM | 20903 | OH2 | WAT | 3973 | -13.103 | 5.510 | 51.486 | 1.00 32.37 |
| MOTA | 20904 | | WAT | 3974 | 35.572 | -38.920 | 31.797 | 1.00 29.21 |
| ATOM | 20905 | | WAT | 3975 | 42.490 | -6.432 | 48.177 | 1.00 37.33 |
| | | | | | | | 19.225 | 1.00 37.33 |
| MOTA | 20906 | OH2 | | 3976 | 55.908 | 7.452 | | |
| MOTA | 20907 | | TAW | 3977 | -23.545 | | -12.731 | 1.00 36.65 |
| ATOM | 20908 | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3978 | | -25.699 | 42.423 | 1.00 28.23 |
| ATOM | 20909 | он2 | WAT | 3979 | 24.546 | 4.768 | 33.624 | 1.00 34.00 |
| ATOM | 20910 | OH2 | TAW | 3980 | 11.846 | -56.638 | 27.547 | 1.00 36.56 |
| ATOM | 20911 | OH2 | WAT | 3981 | -11.970 | -28.236 | 68.101 | 1.00 31.56 |
| ATOM | 20912 | | WAT | 3982 | 34.680 | 0.521 | 51.130 | 1.00 26.18 |
| | 20913 | | WAT | 3983 | 24.960 | -27.638 | 15.617 | 1.00 35.13 |
| ATOM | | | | | | | | |
| MOTA | 20914 | | WAT | 3984 | 12.178 | -47.174 | 31.370 | 1.00 34.11 |
| MOTA | 20915 | | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 3985 | | -29.408 | 25.980 | 1.00 20.06 |
| ATOM | 20916 | OH2 | WAT | 3986 | -5.239 | -4.738 | 26.410 | 1.00 30.64 |
| MOTA | 20917 | OH2 | WAT | 3987 | 7.222 | 25.190 | 72.525 | 1.00 29.80 |
| MOTA | 20918 | OH2 | WAT | 3988 | -8.316 | -17.085 | 4.491 | 1.00 32.12 |
| ATOM | 20919 | | WAT | 3989 | 14.875 | | 62.713 | 1.00 36.51 |
| ATOM | 20920 | | WAT | 3990 | | -32.480 | 35.647 | 1.00 31.85 |
| | | | | | | | 24.647 | 1.00 28.93 |
| ATOM | 20921 | | TAW | 3991 | 26.991 | 6.700 | | |
| MOTA | 20922 | | TAW | 3992 | 9.431 | | 4.689 | 1.00 31.20 |
| ATOM | 20923 | | TAW | 3993 | 23.751 | 35.159 | 59.828 | 1.00 30.73 |
| ATOM | 20924 | OH2 | TAW | 3994 | -29.524 | 4.920 | 48.463 | 1.00 38.77 |
| MOTA | 20925 | OH2 | WAT | 3995 | -10.036 | 20.469 | 3.697 | 1.00 27.33 |
| ATOM | 20926 | OH2 | WAT | 3996 | 13.430 | -13.926 | 30.486 | 1.00 27.55 |
| ATOM | 20927 | | TAW | 3997 | | -30.155 | 4.910 | 1.00 27.29 |
| | 20928 | | WAT | 3998 | -1.861 | 2.934 | 16.906 | 1.00 22.81 |
| MOTA | | | | | | | | |
| MOTA | 20929 | | TAW | 3999 | -6.312 | | 39.194 | 1.00 36.98 |
| MOTA | 20930 | | WAT | 4000 | 0.162 | 16.385 | 31.968 | 1.00 40.85 |
| MOTA | 20931 | OH2 | \mathbf{WAT} | 4001 | 37.331 | -42.808 | 29.079 | 1.00 35.13 |
| MOTA | 20932 | OH2 | TAW | 4002 | 1.728 | 0.651 | 41.556 | 1.00 40.93 |
| MOTA | 20933 | OH2 | TAW | 4003 | 7.955 | -18.489 | -7.241 | 1.00 41.83 |
| MOTA | 20934 | OH2 | WAT | 4004 | -2.324 | ~24.753 | 41.326 | 1.00 36.27 |
| ATOM | 20935 | | WAT | 4005 | -14.001 | -19.794 | -0.066 | 1.00 34.42 |
| MOTA | 20936 | | WAT | 4006 | 19.662 | | | 1.00 32.80 |
| | | | | | | | | |
| MOTA | 20937 | | WAT | 4007 | 10.564 | | | 1.00 29.84 |
| MOTA | 20938 | | TAW | 4008 | 15.113 | 15.031 | 39.754 | 1.00 30.34 |
| MOTA | 20939 | он2 | WAT | 4009 | 35.331 | -21.374 | 20.527 | 1.00 31.28 |
| MOTA | 20940 | OH2 | \mathbf{WAT} | 4010 | 22.819 | 15.879 | 3.191 | 1.00 35.03 |
| ATOM | 20941 | OH2 | WAT | 4011 | -10.543 | -46.147 | 9.362 | 1.00 38.45 |
| ATOM | 20942 | OH2 | WAT | 4012 | -16.594 | 34.561 | 56.964 | 1.00 28.81 |
| ATOM | 20943 | | WAT | 4013 | -10.146 | 32.295 | 63.758 | 1.00 37.29 |
| ATOM | 20944 | | WAT | 4014 | 48.882 | -7.382 | 51.071 | 1.00 37.37 |
| | | | | | | | | |
| MOTA | 20945 | - | TAW | 4015 | 29.920 | 7.293 | 29.541 | 1.00 33.85 |
| ATOM | 20946 | | WAT | 4016 | 19.625 | | 72.073 | 1.00 36.63 |
| ATOM | 20947 | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 4017 | | -34.511 | 37.285 | 1.00 29.54 |
| MOTA | 20948 | OH2 | WAT | 4018 | -5.762 | -7.177 | 29.837 | 1.00 31.23 |
| MOTA | 20949 | OH2 | WAT | 4019 | 11.378 | -38.956 | 13.198 | 1.00 31.14 |
| MOTA | 20950 | | WAT | 4020 | -7.090 | -14.815 | 72.040 | 1.00 26.77 |
| ATOM | 20951 | | WAT | 4021 | 2.252 | 22.804 | -7.049 | 1.00 32.91 |
| MOTA | 20952 | | WAT | 4022 | -3.449 | 14.552 | -24.093 | 1.00 36.29 |
| ATOM | | | WAT | 4022 | -8.112 | 3.142 | -24.672 | 1.00 33.84 |
| | 20953 | | | | | -21.806 | 8.212 | |
| MOTA | 20954 | | WAT | 4024 | 18.026 | | | 1.00 29.93 |
| MOTA | 20955 | | WAT | 4025 | 60.020 | 17.539 | 13.000 | 1.00 44.67 |
| MOTA | 20956 | OH2 | WAT | 4026 | -26.370 | -39.869 | 16.104 | 1.00 41.85 |
| MOTA | 20957 | OH2 | WAT | 4027 | 16.764 | 19.360 | 52.609 | 1.00 28.33 |
| MOTA | 20958 | OH2 | TAW | 4028 | 35.990 | 24.016 | 40.511 | 1.00 34.74 |
| MOTA | 20959 | | WAT | 4029 | 57.458 | 10.198 | 50.817 | 1.00 32.75 |
| ATOM | 20960 | | WAT | 4030 | 1.804 | | 30.519 | 1.00 26.50 |
| ATOM | 20961 | | WAT | 4031 | -10.626 | -9.725 | 72.521 | 1.00 38.53 |
| | | | | | | -27.164 | 51.358 | 1.00 38.33 |
| MOTA | 20962 | | TAW | 4032 | 43.991 | | | |
| MOTA | 20963 | | WAT | 4033 | -28.328 | -39.519 | 17.822 | 1.00 37.78 |
| MOTA | 20964 | | WAT | 4034 | -29.987 | -22.766 | 8.334 | 1.00 31.96 |
| MOTA | 20965 | OH2 | WAT | 4035 | 2.256 | 13.057 | -20.781 | 1.00 40.03 |
| MOTA | 20966 | OH2 | WAT | 4036 | 25.989 | -20.630 | -14.613 | 1.00 32.18 |
| MOTA | 20967 | OH2 | WAT | 4037 | 2.215 | -18.558 | 69.068 | 1.00 34.21 |
| MOTA | 20968 | | WAT | 4038 | -36.511 | | 14.921 | 1.00 29.01 |
| ATOM | 20969 | | WAT | 4039 | 2.072 | 25.410 | 67.667 | 1.00 25.96 |
| MOTA | 20970 | | WAT | 4040 | -4.117 | -40.064 | 35.025 | 1.00 27.36 |
| | | | | | 3.196 | 26.403 | 17.608 | 1.00 27.30 |
| MOTA MOTA | 20971 20972 | | WAT | 4041 | | | | |
| | | いロフ | WAT | 4042 | 4.213 | -11.022 | 21.040 | 1.00 25.61 |

| ATOM | 20973 | OH2 WAT | 4043 | 20.672 | 6.288 | 43.154 | 1.00 11.39 |
|------|----------------|------------|------|---------|---------|---------|------------|
| ATOM | 20974 | OH2 WAT | 4044 | 24.230 | 13.675 | 24.481 | 1.00 17.87 |
| ATOM | 20975 | OH2 WAT | 4045 | | -12.039 | 39.730 | 1.00 16.52 |
| ATOM | 20976 | OH2 WAT | 4046 | | -45.541 | 12.487 | 1.00 25.04 |
| | | | 4047 | 21.124 | 0.639 | 54.913 | 1.00 19.00 |
| ATOM | 20977 | OH2 WAT | | | | | |
| MOTA | 20978 | OH2 WAT | 4048 | | -15.313 | 20.740 | 1.00 17.94 |
| ATOM | 20979 | OH2 WAT | 4049 | 7.082 | 3.993 | 47.118 | 1.00 22.59 |
| MOTA | 20980 | OH2 WAT | 4050 | -15.003 | 20.551 | -11.225 | 1.00 23.46 |
| ATOM | 20981 | OH2 WAT | 4051 | 5.614 | -3.781 | 42.911 | 1.00 18.68 |
| MOTA | 20982 | OH2 WAT | 4052 | 2.878 | -5.383 | 14.276 | 1.00 21.86 |
| ATOM | 20983 | OH2 WAT | 4053 | -28.975 | 0.173 | 43.415 | 1.00 25.48 |
| MOTA | 20984 | OH2 WAT | 4054 | 18.990 | 13.786 | 23.082 | 1.00 34.23 |
| ATOM | 20985 | OH2 WAT | 4055 | 14.863 | 15.999 | 12.872 | 1.00 22.69 |
| ATOM | 20986 | OH2 WAT | 4056 | | -26.590 | 36.835 | 1.00 20.51 |
| ATOM | 20987 | OH2 WAT | 4057 | 16.881 | 17.463 | 50.738 | 1.00 25.65 |
| ATOM | 20988 | OH2 WAT | 4058 | | -15.429 | 23.245 | 1.00 25.72 |
| ATOM | 20989 | OH2 WAT | 4059 | 1.948 | -8.274 | 37.874 | 1.00 24.67 |
| | | OH2 WAT | | -0.846 | 5.377 | 57.566 | 1.00 24.07 |
| ATOM | 20990 | | 4060 | | | | |
| MOTA | 20991 | OH2 WAT | 4061 | | -16.631 | 28.299 | 1.00 26.60 |
| ATOM | 20992 | OH2 WAT | 4062 | 8.670 | -7.127 | 7.982 | 1.00 23.89 |
| MOTA | 20993 | OH2 WAT | 4063 | 7.943 | 4.878 | 13.325 | 1.00 29.72 |
| MOTA | 20994 | OH2 WAT | 4064 | | -18.149 | 38.159 | 1.00 24.67 |
| MOTA | 20995 | OH2 WAT | 4065 | 19.946 | -16.578 | 22.471 | 1.00 21.68 |
| ATOM | 20996 | OH2 WAT | 4066 | 26.755 | -23.578 | 42.730 | 1.00 30.96 |
| MOTA | 20997 | OH2 WAT | 4067 | 19.813 | -21.428 | 77.332 | 1.00 26.96 |
| MOTA | 20998 | OH2 WAT | 4068 | -14.611 | -27.813 | 24.596 | 1.00 22.85 |
| ATOM | 20999 | OH2 WAT | 4069 | 10.556 | -42.741 | 36.183 | 1.00 30.39 |
| ATOM | 21000 | OH2 WAT | 4070 | 9.656 | 11.940 | 15.495 | 1.00 33.39 |
| ATOM | 21001 | OH2 WAT | 4071 | 15.586 | -6.472 | 42.294 | 1.00 26.75 |
| | 21001 | OH2 WAT | 4072 | 21.817 | 15.587 | 28.120 | 1.00 36.02 |
| MOTA | | | | | | | 1.00 30.62 |
| MOTA | 21003 | OH2 WAT | 4073 | | -29.610 | 52.935 | |
| ATOM | 21004 | OH2 WAT | 4074 | | -46.625 | 9.621 | 1.00 25.65 |
| ATOM | 21005 | OH2 WAT | 4075 | | -39.337 | 16.988 | 1.00 29.68 |
| MOTA | 21006 | OH2 WAT | 4076 | 12.558 | 54.160 | 17.405 | 1.00 42.52 |
| ATOM | 21007 | OH2 WAT | 4077 | | -21.050 | -8.217 | 1.00 35.25 |
| MOTA | 21008 | OH2 WAT | 4078 | 14.627 | -21.292 | 77.322 | 1.00 26.15 |
| MOTA | 21009 | OH2 WAT | 4079 | 38.511 | 12.796 | 27.817 | 1.00 32.17 |
| ATOM | 21010 | OH2 WAT | 4080 | 6.634 | -11.234 | 41.030 | 1.00 33.51 |
| ATOM | 21011 | OH2 WAT | 4081 | 19.800 | 4.002 | -7.345 | 1.00 31.84 |
| ATOM | 21012 | OH2 WAT | 4082 | -11.712 | | -16.297 | 1.00 37.20 |
| ATOM | 21013 | OH2 WAT | 4083 | -1.181 | | -23.740 | 1.00 27.77 |
| ATOM | 21013 | OH2 WAT | 4084 | -13.478 | 31.890 | 22.898 | 1.00 35.63 |
| | | | | -26.720 | -9.960 | 27.431 | 1.00 33.03 |
| ATOM | 21015 | OH2 WAT | 4085 | | | | |
| MOTA | 21016 | OH2 WAT | 4086 | | -27.440 | 21.028 | 1.00 46.92 |
| MOTA | 21017 | OH2 WAT | 4087 | | -19.353 | | 1.00 22.71 |
| MOTA | 21018 | OH2 WAT | 4088 | 12.468 | -6.264 | 66.043 | 1.00 33.46 |
| MOTA | 21019 | OH2 WAT | 4089 | | -36.608 | 12.813 | 1.00 30.40 |
| ATOM | 21020 | OH2 WAT | 4090 | 31.960 | -4.177 | 33.906 | 1.00 33.61 |
| ATOM | 21021 | OH2 WAT | 4091 | 7.583 | -54.047 | 28.356 | 1.00 26.52 |
| ATOM | 21022 | OH2 WAT | 4092 | 0.614 | 21.888 | 44.748 | 1.00 35.94 |
| MOTA | 21023 | OH2 WAT | 4093 | 37.538 | -5.989 | 37.641 | 1.00 32.64 |
| ATOM | 21024 | OH2 WAT | 4094 | 21.638 | | 39.740 | 1.00 17.05 |
| ATOM | 21025 | OH2 WAT | 4095 | | -46.828 | 32.920 | 1.00 24.39 |
| ATOM | 21026 | OH2 WAT | 4096 | | -19.653 | 5.133 | 1.00 25.49 |
| ATOM | 21020 | OH2 WAT | 4097 | | -44.364 | 8.973 | 1.00 23.49 |
| ATOM | 21027 | OH2 WAT | 4098 | 27.647 | 11.322 | 5.334 | 1.00 37.09 |
| | 21028 | | | | | | 1.00 32.90 |
| ATOM | | OH2 WAT | 4099 | | -49.393 | 8.411 | |
| ATOM | 21030 | OH2 WAT | 4100 | | -39.224 | 10.206 | 1.00 32.32 |
| ATOM | 21031 | OH2 WAT | 4101 | | -40.087 | 37.856 | 1.00 50.14 |
| ATOM | 21032 | | 4102 | -24.342 | -7.153 | 30.038 | 1.00 30.58 |
| ATOM | 21033 | OH2 WAT | 4103 | -0.619 | 11.724 | -26.102 | 1.00 35.65 |
| ATOM | 21034 | OH2 WAT | 4104 | -9.425 | 29.111 | 31.719 | 1.00 37.15 |
| MOTA | 21035 | OH2 WAT | 4105 | | -16.675 | 32.368 | 1.00 36.40 |
| MOTA | 21036 | OH2 WAT | 4106 | 14.318 | 14.720 | 0.095 | 1.00 27.76 |
| ATOM | 21037 | OH2 WAT | 4107 | 46.641 | -18.008 | 5.068 | 1.00 28.99 |
| ATOM | 21038 | OH2 WAT | 4108 | 40.504 | -35.415 | 30.077 | 1.00 30.68 |
| ATOM | | OH2 WAT | 4109 | -21.465 | 1.072 | -0.752 | 1.00 33.32 |
| ATOM | 21040 | OH2 WAT | 4110 | 46.498 | -3.634 | 42.684 | 1.00 31.74 |
| ATOM | 21040 | OH2 WAT | 4111 | | -56.294 | 21.233 | 1.00 25.38 |
| ATOM | 21041 | OH2 WAT | 4112 | | -54.443 | 22.412 | 1.00 25.38 |
| | | | | | | | 1.00 30.18 |
| ATOM | 21043 | OH2 WAT | 4113 | | -12.430 | 3.805 | |
| ATOM | 21044 | OH2 WAT | 4114 | | -33.290 | 16.444 | 1.00 31.75 |
| ATOM | 21045 | OH2 WAT | 4115 | 26.923 | 26.631 | 13.935 | 1.00 33.99 |
| ATOM | 21046 | OH2 WAT | 4116 | -29.043 | 5.487 | -7.898 | 1.00 45.43 |
| ATOM | | OTTO LIBER | 4117 | -16.588 | -19.270 | 41.769 | 1.00 31.95 |
| | 21047 | OH2 WAT | | | | | |
| MOTA | 21047 21048 | OH2 WAT | 4118 | 6.070 | 9.092 | 39.715 | 1.00 30.14 |
| | | | | 6.070 | | | |

| ATOM | 21050 | OH2 WAT | 4120 | 52.126 | -3.822 | 53.340 | 1.00 45.42 |
|------|-------|----------------|------|---------|----------------|---------|------------|
| ATOM | 21051 | OH2 WAT | 4121 | 46.817 | | -14.025 | 1.00 46.99 |
| ATOM | 21052 | OH2 WAT | 4122 | -12.592 | 3.190 | 66.991 | 1.00 35.76 |
| ATOM | 21052 | OH2 WAT | 4123 | 3.350 | 29.034 | 35.859 | 1.00 34.34 |
| | | | 4124 | 0.606 | -33.642 | 55.873 | 1.00 32.91 |
| ATOM | 21054 | OH2 WAT | | | | | |
| MOTA | 21055 | OH2 WAT | 4125 | -14.891 | 36.065 | 20.896 | 1.00 37.79 |
| MOTA | 21056 | OH2 WAT | 4126 | -25.092 | 9.956 | 50.529 | 1.00 32.04 |
| MOTA | 21057 | OH2 WAT | 4127 | 24.645 | 3.578 | 21.558 | 1.00 33.84 |
| MOTA | 21058 | OH2 WAT | 4128 | 14.966 | -15.407 | 27.047 | 1.00 37.48 |
| ATOM | 21059 | OH2 WAT | 4129 | 25.311 | 0.590 | 59.424 | 1.00 32.26 |
| ATOM | 21060 | OH2 WAT | 4130 | 5.921 | 2.186 | 48.638 | 1.00 28.21 |
| ATOM | 21061 | OH2 WAT | 4131 | | -33.527 | 6.693 | 1.00 29.78 |
| ATOM | 21062 | OH2 WAT | 4132 | -9.038 | 35.946 | 43.790 | 1.00 37.55 |
| ATOM | 21063 | OH2 WAT | 4133 | 17.435 | -31.315 | 16.469 | 1.00 31.72 |
| ATOM | 21064 | OH2 WAT | 4134 | 30.359 | 5.569 | 52.711 | 1.00 23.92 |
| ATOM | 21065 | OH2 WAT | 4135 | | -12.556 | 17.583 | 1.00 19.93 |
| ATOM | 21066 | OH2 WAT | 4136 | | -23.653 | 47.102 | 1.00 24.33 |
| | 21067 | OH2 WAT | 4137 | 4.278 | 27.765 | 15.197 | 1.00 31.50 |
| ATOM | | | | | -15.894 | 41.477 | 1.00 20.38 |
| ATOM | 21068 | OH2 WAT | 4138 | | | | 1.00 20.38 |
| ATOM | 21069 | OH2 WAT | 4139 | 28.301 | -2.532 | -0.522 | |
| ATOM | 21070 | OH2 WAT | 4140 | | -34.367 | 20.394 | 1.00 26.22 |
| ATOM | 21071 | OH2 WAT | 4141 | -17.982 | 10.709 | 12.655 | 1.00 28.44 |
| ATOM | 21072 | OH2 WAT | 4142 | | -13.857 | 17.205 | 1.00 25.59 |
| ATOM | 21073 | OH2 WAT | 4143 | | -15.812 | 37.733 | 1.00 25.27 |
| ATOM | 21074 | OH2 WAT | 4144 | | -19.299 | 7.566 | 1.00 26.09 |
| MOTA | 21075 | OH2 WAT | 4145 | 9.956 | -49.449 | 29.174 | 1.00 28.96 |
| ATOM | 21076 | OH2 WAT | 4146 | 17.480 | 3.336 | 10.956 | 1.00 30.39 |
| MOTA | 21077 | OH2 WAT | 4147 | 8.517 | -4.567 | 9.940 | 1.00 31.22 |
| ATOM | 21078 | OH2 WAT | 4148 | -7.175 | 0.887 | 19.891 | 1.00 27.12 |
| ATOM | 21079 | OH2 WAT | 4149 | 28.989 | 41.203 | 15.263 | 1.00 29.63 |
| ATOM | 21080 | OH2 WAT | 4150 | 23.580 | 3.660 | 40.283 | 1.00 39.46 |
| ATOM | 21081 | OH2 WAT | 4151 | 13.879 | 13.838 | 16.264 | 1.00 28.18 |
| ATOM | 21082 | OH2 WAT | 4152 | 3.363 | -53.015 | 26.505 | 1.00 26.41 |
| | | OH2 WAT | 4153 | | -31.794 | 51.912 | 1.00 29.88 |
| ATOM | 21083 | | | | | | |
| ATOM | 21084 | OH2 WAT | 4154 | 15.462 | 21.257 | 30.971 | 1.00 33.63 |
| MOTA | 21085 | OH2 WAT | 4155 | | -11.032 | 37.773 | 1.00 32.69 |
| MOTA | 21086 | OH2 WAT | 4156 | 4.765 | -2.386 | 40.740 | 1.00 35.83 |
| MOTA | 21087 | OH2 WAT | 4157 | | -19.667 | 75.203 | 1.00 37.72 |
| MOTA | 21088 | OH2 WAT | 4158 | | -11.102 | 19.527 | 1.00 33.73 |
| MOTA | 21089 | OH2 WAT | 4159 | -1.263 | 16.009 | 20.936 | 1.00 27.24 |
| MOTA | 21090 | OH2 WAT | 4160 | -6.256 | -45.054 | 6.939 | 1.00 41.51 |
| MOTA | 21091 | OH2 WAT | 4161 | 15.761 | -28.451 | 54.807 | 1.00 36.09 |
| MOTA | 21092 | OH2 WAT | 4162 | 18.439 | 14.295 | 19.227 | 1.00 38.49 |
| ATOM | 21093 | OH2 WAT | 4163 | -3.972 | -20.387 | 37.814 | 1.00 31.16 |
| ATOM | 21094 | OH2 WAT | 4164 | 18.013 | -1.645 | 54.687 | 1.00 30.47 |
| ATOM | 21095 | OH2 WAT | 4165 | -15.633 | 33.909 | 22.604 | 1.00 31.22 |
| ATOM | 21096 | OH2 WAT | 4166 | 40.780 | -8.375 | 40.145 | 1.00 32.51 |
| ATOM | 21097 | OH2 WAT | 4167 | 47.802 | 30.040 | 7.228 | 1.00 40.79 |
| ATOM | 21098 | OH2 WAT | 4168 | -3.032 | -32.860 | 34.864 | 1.00 27.66 |
| ATOM | | | | | | | |
| | 21099 | OH2 WAT | 4169 | 9.198 | 20.743 | 72.320 | 1.00 35.07 |
| ATOM | 21100 | OH2 WAT | 4170 | | -21.527 | 2.995 | 1.00 36.62 |
| ATOM | 21101 | OH2 WAT | 4171 | | -6.086 | | |
| MOTA | 21102 | OH2 WAT | 4172 | | -11.466 | 53.111 | 1.00 44.39 |
| MOTA | 21103 | OH2 WAT | 4173 | | -20.387 | 40.817 | 1.00 30.20 |
| MOTA | 21104 | OH2 WAT | 4174 | -10.618 | -14.092 | 4.622 | 1.00 31.64 |
| ATOM | 21105 | OH2 WAT | 4175 | | -19.755 | 5.914 | 1.00 37.61 |
| MOTA | 21106 | OH2 WAT | 4176 | 19.353 | -22.226 | 0.817 | 1.00 32.55 |
| ATOM | 21107 | OH2 WAT | 4177 | -29.776 | -5.355 | 39.885 | 1.00 30.32 |
| ATOM | 21108 | OH2 WAT | 4178 | | -13.068 | | 1.00 35.70 |
| ATOM | 21109 | OH2 WAT | 4179 | -8.062 | 5.216 | 33.169 | 1.00 25.98 |
| ATOM | 21110 | OH2 WAT | 4180 | -2.522 | 30.394 | 63.742 | 1.00 28.47 |
| ATOM | 21111 | OH2 WAT | 4181 | 46.009 | 3.328 | 33.070 | 1.00 35.13 |
| ATOM | 21112 | OH2 WAT | 4182 | 8.360 | 8.234 | 41.757 | 1.00 33.13 |
| ATOM | 21113 | OH2 WAT | 4183 | | -18.598 | 55.686 | 1.00 23.10 |
| | 21113 | | | -16.001 | 22.656 | | |
| ATOM | | OH2 WAT | 4184 | | | 38.987 | 1.00 29.36 |
| ATOM | 21115 | OH2 WAT | 4185 | | -36.135 | 10.535 | 1.00 37.88 |
| ATOM | 21116 | OH2 WAT | 4186 | -15.684 | -9.143 | -8.092 | 1.00 31.91 |
| ATOM | 21117 | OH2 WAT | 4187 | -1.090 | 1.204 | 14.459 | 1.00 30.11 |
| ATOM | 21118 | OH2 WAT | 4188 | 44.289 | 2.682 | 29.166 | 1.00 28.69 |
| ATOM | 21119 | OH2 WAT | 4189 | | -28.362 | 46.000 | 1.00 28.10 |
| MOTA | 21120 | OH2 WAT | 4190 | 13.135 | -5.781 | 41.932 | 1.00 35.53 |
| MOTA | 21121 | OH2 WAT | 4191 | 19.734 | 30.686 | 49.844 | 1.00 35.70 |
| ATOM | 21122 | OH2 WAT | 4192 | -36.378 | -21.364 | 23.565 | 1.00 35.60 |
| ATOM | 21123 | OH2 WAT | 4193 | 17.251 | 0.350 | 12.314 | 1.00 23.98 |
| ATOM | 21124 | OH2 WAT | 4194 | -10.271 | -38.090 | 23.438 | 1.00 32.22 |
| ATOM | 21125 | OH2 WAT | 4195 | -22.687 | 7.954 | 3.699 | 1.00 33.28 |
| ATOM | 21126 | OH2 WAT | 4196 | -21.951 | 15.459 | 4.933 | 1.00 31.65 |
| - | · | · - | | | · - | | |

| ATOM | 21127 | OH2 W | TAV | 4197 | -17.403 | 21.503 | -8.388 | 1.00 32.40 |
|------|-------|-------|-----|------|---------|---------|---------|------------|
| ATOM | 21128 | OH2 W | TAV | 4198 | 21.977 | 9.231 | 37.108 | 1.00 32.87 |
| ATOM | 21129 | | | 4199 | 37.419 | 17.868 | 21.884 | 1.00 46.31 |
| ATOM | 21130 | OH2 W | | 4200 | 22.196 | 9.629 | 18.773 | 1.00 31.77 |
| MOTA | 21131 | OH2 W | | 4201 | 16.692 | -23.322 | -5.245 | 1.00 36.91 |
| ATOM | 21132 | OH2 V | | 4202 | 42.777 | -33.719 | 53.939 | 1.00 35.86 |
| | | OH2 V | | 4203 | 1.354 | -2.239 | 14.757 | 1.00 37.10 |
| ATOM | 21133 | | | | | | | 1.00 37.10 |
| ATOM | 21134 | OH2 V | | 4204 | -26.952 | -3.544 | 38.440 | |
| ATOM | 21135 | | | 4205 | 29.239 | -5.609 | 38.042 | 1.00 29.97 |
| MOTA | 21136 | | | 4206 | 43.138 | 0.368 | 25.089 | 1.00 32.24 |
| ATOM | 21137 | OH2 V | | 4207 | 52.415 | -7.788 | 51.945 | 1.00 30.80 |
| MOTA | 21138 | OH2 V | TAV | 4208 | -2.220 | 0.196 | 40.301 | 1.00 41.13 |
| MOTA | 21139 | OH2 V | TAN | 4209 | 9.166 | -36.364 | 8.279 | 1.00 32.28 |
| MOTA | 21140 | OH2 V | TAV | 4210 | 37.549 | -23.883 | 19.085 | 1.00 35.85 |
| ATOM | 21141 | OH2 V | TAV | 4211 | 40.366 | -43.408 | 18.178 | 1.00 35.18 |
| ATOM | 21142 | OH2 V | TAN | 4212 | 41.259 | -39.426 | 17.720 | 1.00 35.03 |
| ATOM | 21143 | | | 4213 | 5.966 | -16.794 | 26.485 | 1.00 33.99 |
| ATOM | 21144 | | | 4214 | -0.504 | 24.436 | 38.709 | 1.00 31.34 |
| MOTA | 21145 | | | 4215 | -31.816 | -7.311 | 63.265 | 1.00 46.67 |
| MOTA | 21146 | | | 4216 | | -27.488 | 41.591 | 1.00 32.87 |
| | | | | 4217 | 22.491 | 8.396 | 33.548 | 1.00 37.01 |
| ATOM | 21147 | OH2 V | | | | | | 1.00 34.59 |
| MOTA | 21148 | | | 4218 | 8.588 | 14.998 | -7.928 | |
| MOTA | 21149 | | | 4219 | -5.071 | 39.648 | 64.146 | 1.00 36.17 |
| MOTA | 21150 | | | 4220 | 30.649 | 7.956 | 54.006 | 1.00 28.56 |
| MOTA | 21151 | | | 4221 | -25.150 | 4.421 | 48.986 | 1.00 31.32 |
| ATOM | 21152 | OH2 V | | 4222 | 4.603 | -15.946 | 39.930 | 1.00 28.11 |
| ATOM | 21153 | OH2 V | TAN | 4223 | -19.155 | 22.017 | 52.855 | 1.00 36.51 |
| MOTA | 21154 | OH2 V | TAN | 4224 | -1.225 | 27.223 | 40.496 | 1.00 34.03 |
| ATOM | 21155 | OH2 V | TAN | 4225 | 9.323 | -6.838 | 44.620 | 1.00 32.56 |
| MOTA | 21156 | OH2 V | TAN | 4226 | -13.348 | -40.907 | 25.217 | 1.00 36.02 |
| ATOM | 21157 | OH2 V | | 4227 | -29.811 | -16.829 | 55.472 | 1.00 40.39 |
| ATOM | 21158 | OH2 V | | 4228 | 1.208 | | -12.804 | 1.00 25.50 |
| ATOM | 21159 | OH2 V | | 4229 | 31.515 | 42.188 | 14.797 | 1.00 36.19 |
| ATOM | 21160 | OH2 V | | 4230 | | -40.140 | 8.269 | 1.00 32.85 |
| | | | | | 4.884 | -8.621 | 38.037 | 1.00 32.03 |
| MOTA | 21161 | | | 4231 | | | | 1.00 23.37 |
| MOTA | 21162 | OH2 V | | 4232 | | -12.337 | 43.000 | |
| MOTA | 21163 | | | 4233 | 22.346 | 33.851 | 68.574 | 1.00 47.30 |
| MOTA | 21164 | OH2 V | | 4234 | 6.737 | 5.652 | 40.043 | 1.00 42.41 |
| MOTA | 21165 | | | 4235 | | -13.093 | 37.173 | 1.00 33.25 |
| MOTA | 21166 | | | 4236 | 5.818 | -1.680 | 14.657 | 1.00 40.01 |
| ATOM | 21167 | OH2 V | WAT | 4237 | -5.653 | -17.045 | 3.161 | 1.00 38.26 |
| MOTA | 21168 | OH2 V | MAT | 4238 | -22.623 | 5.252 | 41.872 | 1.00 32.25 |
| MOTA | 21169 | OH2 V | TAN | 4239 | -13.321 | -28.124 | 62.372 | 1.00 31.95 |
| ATOM | 21170 | OH2 V | TAW | 4240 | -22.968 | -6.416 | 35.146 | 1.00 22.64 |
| MOTA | 21171 | OH2 V | TAW | 4241 | -27.579 | -29.214 | 23.224 | 1.00 28.40 |
| MOTA | 21172 | | | 4242 | -17.589 | -1.229 | 71.448 | 1.00 40.90 |
| ATOM | 21173 | | | 4243 | | -26.804 | 3.938 | 1.00 30.62 |
| ATOM | 21174 | | | 4244 | | -44.495 | 29.557 | 1.00 40.76 |
| ATOM | 21175 | | | 4245 | -4.840 | 12.652 | 24.363 | 1.00 35.77 |
| ATOM | 21176 | | | 4246 | 47.599 | -6.430 | 55.516 | 1.00 36.89 |
| | | OH2 V | | | -28.043 | 2.899 | -0.586 | 1.00 42.68 |
| MOTA | 21177 | | | 4247 | | | | |
| ATOM | 21178 | OH2 V | | 4248 | | -37.649 | 16.094 | 1.00 42.67 |
| MOTA | 21179 | | | 4249 | 22.684 | 29.859 | 5.493 | 1.00 39.59 |
| MOTA | 21180 | | | 4250 | -8.757 | 40.956 | 1.091 | 1.00 32.81 |
| MOTA | 21181 | | | 4251 | 40.067 | -45.503 | 20.265 | 1.00 35.71 |
| MOTA | 21182 | | | 4252 | 26.027 | 1.180 | 40.411 | 1.00 31.92 |
| MOTA | 21183 | OH2 V | | 4253 | 17.254 | -13.580 | 32.677 | 1.00 37.95 |
| MOTA | 21184 | OH2 V | TAW | 4254 | 38.172 | 16.681 | 33.750 | 1.00 36.90 |
| MOTA | 21185 | OH2 V | WAT | 4255 | -23.882 | 11.970 | 4.626 | 1.00 35.75 |
| ATOM | 21186 | OH2 V | TAW | 4256 | 24.484 | 29.594 | 17.149 | 1.00 36.63 |
| ATOM | 21187 | OH2 V | WAT | 4257 | 14.330 | 14.056 | -7.663 | 1.00 32.35 |
| MOTA | 21188 | OH2 V | WAT | 4258 | 9.933 | -26.844 | 55.259 | 1.00 34.01 |
| MOTA | 21189 | | | 4259 | 12.646 | -9.356 | -24.468 | 1.00 43.12 |
| ATOM | 21190 | | | 4260 | 40.273 | -5.490 | 1.123 | 1.00 31.20 |
| MOTA | 21191 | | | 4261 | 17.384 | -0.963 | 15.304 | 1.00 40.38 |
| ATOM | 21192 | | | 4262 | 7.357 | 1.338 | 55.482 | 1.00 34.09 |
| | 21192 | | | 4263 | -7.701 | 28.368 | 40.512 | 1.00 31.74 |
| ATOM | | | | | 6.424 | 28.970 | 12.284 | 1.00 31.74 |
| ATOM | 21194 | | | 4264 | | | | 1.00 35.75 |
| MOTA | 21195 | OH2 V | | 4265 | 28.293 | -7.969 | 59.997 | |
| MOTA | 21196 | | | 4266 | 33.471 | -50.990 | 21.231 | 1.00 34.39 |
| ATOM | 21197 | | | 4267 | 36.422 | 1.406 | 67.198 | 1.00 37.21 |
| ATOM | 21198 | | | 4268 | 4.155 | 15.109 | 20.451 | 1.00 40.58 |
| MOTA | 21199 | | | 4269 | -26.153 | -3.024 | -4.695 | 1.00 24.77 |
| MOTA | 21200 | | | 4270 | 30.499 | -25.454 | 72.705 | 1.00 38.88 |
| MOTA | 21201 | | TAW | 4271 | 4.763 | 51.788 | 4.914 | 1.00 27.90 |
| MOTA | 21202 | OH2 V | TAW | 4272 | -11.498 | 46.346 | 14.162 | 1.00 32.61 |
| MOTA | 21203 | OH2 V | WAT | 4273 | 39.036 | -19.110 | 16.994 | 1.00 32.98 |

| ATOM | 21204 | он2 | WAT | 4274 | -6.998 | 36.928 | 26.870 | 1.00 43.35 |
|--------------|----------------|-----|----------------|--------------|-------------------|------------------|------------------|--------------------------|
| MOTA | 21205 | он2 | WAT | 4275 | 46.948 | 7.501 | 34.599 | 1.00 24.81 |
| ATOM | 21206 | OH2 | | 4276 | 50.983 | -8.055 | -5.708 | 1.00 40.55 |
| MOTA | 21207 | ОН2 | | 4277 | 19.452 | -39.708 | 61.023 | 1.00 34.30 |
| MOTA | 21208 | OH2 | | 4278 | 7.397 | -30.621 | 39.404 | 1.00 33.65 |
| ATOM | 21209 | OH2 | | 4279 | 13.876 | -1.133 | 12.109 | 1.00 41.50 |
| ATOM | 21210 | | WAT | 4280 | -0.160 | 20.020 | -0.572 | 1.00 32.16 |
| ATOM | 21211 | OH2 | | 4281 | 45.793 | -19.678 | 50.360 | 1.00 35.75 |
| | 21212 | OH2 | | 4282 | 47.155 | 27.281 | 14.452 | 1.00 38.21 |
| MOTA | | OH2 | | 4283 | 8.531 | -12.525 | 69.846 | 1.00 42.83 |
| MOTA | 21213 | OH2 | | | 38.230 | 21.846 | 69.235 | 1.00 42.03 |
| MOTA | 21214 | | | 4284 | | -15.553 | 2.722 | 1.00 34.37 |
| MOTA | 21215 | OH2 | | 4285 | 49.714 | | | |
| MOTA | 21216 | OH2 | | 4286 | 8.106 | 30.082 32.218 | 54.050 50.889 | 1.00 33.73 |
| MOTA | 21217 | OH2 | | 4287 | 23.244 | | | 1.00 33.29 |
| MOTA | 21218 | OH2 | | 4288 | 17.581 | 21.404 | 35.067 | 1.00 43.77 |
| MOTA | 21219 | OH2 | | 4289 | 19.334 | 9.501 | 37.368 | 1.00 34.18 |
| MOTA | 21220 | OH2 | | 4290 | -32.573 | -19.162 | 54.321 | 1.00 42.08 |
| MOTA | 21221 | OH2 | | 4291 | 36.584 | -48.023 | 13.443 | 1.00 37.99 |
| MOTA | 21222 | OH2 | | 4292 | 53.608 | 2.609 | 45.918 | 1.00 29.33 |
| MOTA | 21223 | он2 | | 4293 | -28.355 | -3.724 | 11.537 | 1.00 36.13 |
| MOTA | 21224 | OH2 | | 4294 | 29.801 | 34.256 | 66.452 | 1.00 42.75 |
| MOTA | 21225 | | \mathbf{v} | 4295 | 37.391 | 14.555 | 21.327 | 1.00 29.90 |
| MOTA | 21226 | OH2 | WAT | 4296 | -0.961 | 22.126 | 13.597 | 1.00 30.11 |
| MOTA | 21227 | OH2 | WAT | 4297 | 31.707 | | -19.155 | 1.00 40.22 |
| MOTA | 21228 | OH2 | \mathbf{WAT} | 4298 | 31.457 | -20.855 | | 1.00 37.42 |
| ATOM | 21229 | OH2 | WAT | 4299 | 25.101 | -17.682 | -14.424 | 1.00 32.68 |
| ATOM · | 21230 | OH2 | WAT | 4300 | 20.756 | 8.915 | -7.538 | 1.00 38.06 |
| ATOM | 21231 | OH2 | WAT | 4301 | 8.289 | -46.227 | 33.339 | 1.00 36.23 |
| ATOM | 21232 | OH2 | WAT | 4302 | -30.592 | -2.404 | 23.454 | 1.00 36.26 |
| ATOM | 21233 | OH2 | WAT | 4303 | -0.554 | 12.427 | -16.863 | 1.00 29.01 |
| MOTA | 21234 | OH2 | WAT | 4304 | 30.322 | -21.630 | -20.939 | 1.00 33.55 |
| MOTA | 21235 | он2 | WAT | 4305 | -15.891 | 14.303 | 49.053 | 1.00 41.02 |
| MOTA | 21236 | он2 | WAT | 4306 | -5.861 | -24.996 | 39.922 | 1.00 37.54 |
| ATOM | 21237 | он2 | WAT | 4307 | -18.592 | 5.594 | 59.709 | 1.00 44.08 |
| ATOM | 21238 | OH2 | WAT | 4308 | -13.782 | -29.666 | 2.092 | 1.00 36.94 |
| | 21239 | | WAT | 4309 | -0.006 | 10.614 | 60.001 | 1.00 43.52 |
| АТОМ | 21240 | OH2 | | 4310 | 32.762 | | -23.904 | 1.00 33.22 |
| ATOM | 21241 | | WAT | 4311 | 38.244 | -3.752 | 7.396 | 1.00 36.21 |
| ATOM | 21242 | | WAT | 4312 | 46.881 | -21.498 | -8.257 | 1.00 46.78 |
| ATOM | 21243 | OH2 | | 4313 | 29.381 | -44.133 | 36.141 | 1.00 38.69 |
| ATOM | 21244 | OH2 | | 4314 | 44.697 | -1.657 | 57.305 | 1.00 27.49 |
| ATOM | 21245 | OH2 | | 4315 | 3.764 | -16.191 | 73.425 | 1.00 46.00 |
| ATOM | 21246 | OH2 | | 4316 | 1.552 | 2.561 | 15.840 | 1.00 39.61 |
| MOTA | 21247 | OH2 | | 4317 | 22.489 | 10.399 | 26.199 | 1.00 41.03 |
| MOTA | 21248 | OH2 | | 4318 | -28.455 | -3.493 | 20.182 | 1.00 29.54 |
| ATOM | 21249 | OH2 | | 4319 | 22.485 | -54.018 | 16.709 | 1.00 30.01 |
| ATOM | 21250 | OH2 | | 4320 | 17.660 | -27.711 | | 1.00 38.58 |
| ATOM | 21251 | OH2 | | 4321 | 56.912 | 13.287 | 51.121 | 1.00 44.62 |
| ATOM | 21252 | OH2 | | 4322 | -21.611 | -37.255 | 5.058 | 1.00 25.63 |
| ATOM | 21252 | OH2 | WAT | 4323 | 36.941 | -3.556 | 52.524 | 1.00 25.05 |
| ATOM | 21254 | OH2 | | 4324 | 13.800 | | -21.931 | 1.00 38.56 |
| ATOM | 21255 | OH2 | | 4325 | | | 18.011 | |
| | 21256 | OH2 | | 4326 | | -32.961 | | 1.00 43.84 |
| ATOM ATOM | 21257 | | WAT | 4327 | 42.719 | 27.673 | 55.936 | 1.00 44.26 |
| | | | | 4327 | 45.545 | 11.091 | 29.384 | 1.00 35.10 |
| MOTA MOTA | 21258 21259 | OH2 | TAW TAW | 4329 | | -50.998 | 23.510 | 1.00 33.10 |
| | 21260 | | | | 37.100 | -20.795 | 16.046 | 1.00 34.18 |
| ATOM | | | WAT WAT | 4330 4331 | | 2.258 | | 1.00 33.51 |
| ATOM ATOM | 21261 21262 | | WAT | 4331 | 22.014 -22.317 | 18.441 | 5.383 | 1.00 35.31 |
| | | OH2 | WAT | | | -27.346 | 26.266 | 1.00 36.71 |
| ATOM | 21263 | | | 4333 | -9.502 | -49.756 | 12.668 | 1.00 25.74 |
| ATOM | 21264 | OH2 | | 4334 | | | | |
| ATOM | 21265 | | WAT | 4335 | | -40.436 | 24.117 | 1.00 33.74 |
| ATOM | 21266 | | WAT | 4336 | -19.836 | | -18.554 | 1.00 46.45 |
| ATOM | 21267 | OH2 | | 4337 | 1.661 | -6.925 | 34.463 | 1.00 36.93 1.00 34.61 |
| MOTA | 21268 | | WAT | 4338 | 42.933 | 18.805 | 72.619 | |
| MOTA | 21269 | | WAT | 4339 | -0.593 | -4.255 | 21.944 | 1.00 32.00 |
| MOTA | | OH2 | | 4340 | 6.393 | 20.185 | 3.149 | 1.00 33.81 |
| MOTA | 21271 | | WAT | 4341 | 15.614 | 24.362 | 5.634 | 1.00 46.42 |
| ATOM | 21272 | | WAT | 4342 | 11.089 | 39.084 | 58.882 | 1.00 38.94 |
| ATOM | 21273 | OH2 | | 4343 | 30.841 | -39.067 | 34.205 | 1.00 44.48 |
| ATOM | 21274 | | WAT | 4344 | 35.060 | -10.488 | 67.360 | 1.00 46.38 |
| MOTA | 21275 | | WAT | 4345 | | -41.917 | 8.912 | 1.00 42.89 |
| ATOM | 21276 | | WAT | 4346 | -10.943 | 42.604 | 43.714 | 1.00 40.74 |
| MOTA | 21277 | OH2 | | 4347 | 16.343 | 51.120 | 19.143 | 1.00 39.64 |
| MOTA | 21278 | | WAT | 4348 | 3.496 | 14.826 | 36.570 | 1.00 28.52 |
| MOTA | 21279 | | WAT | 4349 | 46.266 | 37.133 | 2.322 | 1.00 37.96 |
| MOTA | 21280 | он2 | WAT | 4350 | -11.265 | 42.564 | 22.557 | 1.00 35.16 |

| MOTA | 21281 | OH2 WAT | 4351 | -17.123 | 13.946 | 41.412 | 1.00 37.12 |
|------|-------|---------|------|---------|---------|---------|------------|
| ATOM | 21282 | OH2 WAT | 4352 | -29.129 | -17.466 | 5.755 | 1.00 37.27 |
| ATOM | 21283 | OH2 WAT | 4353 | 31.454 | -25.540 | 69.971 | 1.00 28.84 |
| | | OH2 WAT | 4354 | 29.447 | | -21.989 | 1.00 31.86 |
| ATOM | 21284 | | | | | | |
| ATOM | 21285 | OH2 WAT | 4355 | -16.353 | 12.502 | 47.101 | 1.00 30.21 |
| MOTA | 21286 | OH2 WAT | 4356 | | -13.430 | 21.716 | 1.00 35.82 |
| ATOM | 21287 | OH2 WAT | 4357 | 7.648 | -13.329 | -10.841 | 1.00 33.89 |
| MOTA | 21288 | OH2 WAT | 4358 | 44.573 | 15.736 | 67.094 | 1.00 35.84 |
| ATOM | 21289 | OH2 WAT | 4359 | -12.313 | 23.838 | 12.610 | 1.00 35.05 |
| ATOM | 21290 | OH2 WAT | 4360 | 5.658 | | -23.706 | 1.00 41.15 |
| | | | 4361 | | -30.125 | 22.863 | 1.00 24.72 |
| MOTA | 21291 | OH2 WAT | | | | | 1.00 24.72 |
| MOTA | 21292 | OH2 WAT | 4362 | -5.304 | -48.318 | 25.587 | |
| ATOM | 21293 | OH2 WAT | 4363 | | -35.265 | 45.218 | 1.00 38.38 |
| ATOM | 21294 | OH2 WAT | 4364 | -28.043 | -13.694 | 45.466 | 1.00 34.76 |
| ATOM | 21295 | OH2 WAT | 4365 | 36.395 | -45.668 | 27.357 | 1.00 32.81 |
| ATOM | 21296 | OH2 WAT | 4366 | 45.633 | -16.075 | 9.631 | 1.00 27.97 |
| ATOM | 21297 | OH2 WAT | 4367 | 5.551 | 1.705 | 57.364 | 1.00 37.70 |
| ATOM | 21298 | OH2 WAT | 4368 | 4.335 | 33.487 | 73.208 | 1.00 34.45 |
| | | | | | | | 1.00 39.46 |
| MOTA | 21299 | OH2 WAT | 4369 | -16.577 | | -18.466 | |
| MOTA | 21300 | OH2 WAT | 4370 | 44.958 | -2.975 | 40.294 | 1.00 41.84 |
| MOTA | 21301 | OH2 WAT | 4371 | -11.628 | 28.838 | 13.039 | 1.00 42.95 |
| MOTA | 21302 | OH2 WAT | 4372 | 40.841 | 14.763 | 27.236 | 1.00 45.00 |
| MOTA | 21303 | OH2 WAT | 4373 | 10.333 | 28.827 | 73.761 | 1.00 37.30 |
| ATOM | 21304 | OH2 WAT | 4374 | 1.040 | 49.430 | 3.854 | 1.00 40.14 |
| ATOM | 21305 | OH2 WAT | 4375 | 16.228 | 2.460 | -24.363 | 1.00 29.98 |
| | | | 4376 | -10.817 | | 26.234 | 1.00 28.48 |
| MOTA | 21306 | OH2 WAT | | | | | |
| MOTA | 21307 | OH2 WAT | 4377 | -13.169 | -26.151 | 69.385 | 1.00 42.50 |
| ATOM | 21308 | OH2 WAT | 4378 | 17.911 | -12.633 | 35.282 | 1.00 30.10 |
| MOTA | 21309 | OH2 WAT | 4379 | 9.833 | -18.262 | -5.406 | 1.00 33.81 |
| ATOM | 21310 | OH2 WAT | 4380 | -23.233 | -9.084 | 34.300 | 1.00 30.72 |
| ATOM | 21311 | OH2 WAT | 4381 | 52.131 | 29.747 | 28.709 | 1.00 41.21 |
| ATOM | 21312 | OH2 WAT | 4382 | 1.375 | 6.960 | 58.261 | 1.00 35.75 |
| ATOM | 21312 | OH2 WAT | 4383 | -31.130 | -3.570 | 19.795 | 1.00 39.36 |
| | | | | | | | 1.00 33.30 |
| ATOM | 21314 | OH2 WAT | 4384 | 37.817 | 3.006 | 69.575 | |
| MOTA | 21315 | она жат | 4385 | -4.563 | -16.096 | 0.551 | 1.00 37.46 |
| MOTA | 21316 | OH2 WAT | 4386 | 4.037 | -3.919 | 18.274 | 1.00 32.56 |
| MOTA | 21317 | OH2 WAT | 4387 | -21.141 | -1.984 | 26.707 | 1.00 33.58 |
| ATOM | 21318 | OH2 WAT | 4388 | -22.717 | 1.730 | -11.319 | 1.00 44.33 |
| ATOM | 21319 | OH2 WAT | 4389 | 38.993 | -41.394 | 21.353 | 1.00 26.94 |
| ATOM | 21320 | OH2 WAT | 4390 | 35.457 | -6.585 | 23.306 | 1.00 41.41 |
| ATOM | 21321 | OH2 WAT | 4391 | -28.515 | -11.015 | 44.907 | 1.00 44.09 |
| | | | | | | | 1.00 33.81 |
| MOTA | 21322 | OH2 WAT | 4392 | 21.162 | 12.941 | 61.076 | |
| ATOM | 21323 | OH2 WAT | 4393 | -15.197 | 2.825 | 26.060 | 1.00 39.04 |
| ATOM | 21324 | OH2 WAT | 4394 | -15.450 | -25.101 | 26.034 | 1.00 25.87 |
| ATOM | 21325 | OH2 WAT | 4395 | 2.390 | 19.780 | -0.161 | 1.00 34.76 |
| ATOM | 21326 | OH2 WAT | 4396 | 43.487 | -25.747 | 59.438 | 1.00 35.57 |
| ATOM | 21327 | OH2 WAT | 4397 | 48.629 | 36.856 | 21.672 | 1.00 44.39 |
| ATOM | 21328 | OH2 WAT | 4398 | 17.100 | 12.356 | 40.201 | 1.00 40.21 |
| ATOM | 21329 | OH2 WAT | 4399 | 4.507 | | | 1.00 39.12 |
| | | | | | | 0.821 | |
| MOTA | 21330 | OH2 WAT | 4400 | -27.080 | 5.572 | | 1.00 39.35 |
| MOTA | 21331 | OH2 WAT | 4401 | -3.672 | 0.984 | 37.698 | 1.00 39.93 |
| MOTA | 21332 | OH2 WAT | 4402 | -20.583 | | 49.997 | 1.00 34.01 |
| MOTA | 21333 | OH2 WAT | 4403 | 39.072 | -14.613 | 58.597 | 1.00 31.42 |
| ATOM | 21334 | OH2 WAT | 4404 | 29.709 | 12.185 | 3.398 | 1.00 44.25 |
| ATOM | 21335 | OH2 WAT | 4405 | 35.880 | -22.841 | 12.910 | 1.00 33.52 |
| ATOM | 21336 | OH2 WAT | 4406 | -35.845 | -12.885 | 22.300 | 1.00 34.99 |
| ATOM | 21337 | OH2 WAT | 4407 | 15.319 | 26.997 | 5.574 | 1.00 32.51 |
| | 21338 | OH2 WAT | 4408 | 8.333 | 17.040 | 3.228 | 1.00 40.92 |
| ATOM | | | | -10.936 | | | 1.00 37.53 |
| ATOM | 21339 | OH2 WAT | 4409 | | 26.210 | 13.895 | |
| MOTA | 21340 | OH2 WAT | 4410 | 55.583 | 6.631 | 16.381 | 1.00 45.01 |
| MOTA | 21341 | OH2 WAT | 4411 | 27.248 | -0.852 | 16.193 | 1.00 32.03 |
| MOTA | 21342 | OH2 WAT | 4412 | 11.166 | -30.270 | 54.430 | 1.00 35.34 |
| MOTA | 21343 | OH2 WAT | 4413 | 27.193 | 30.827 | 45.265 | 1.00 48.03 |
| ATOM | 21344 | OH2 WAT | 4414 | 1.816 | -4.001 | 33.376 | 1.00 38.02 |
| ATOM | 21345 | OH2 WAT | 4415 | -7.358 | 6.238 | 21.426 | 1.00 31.68 |
| MOTA | 21346 | OH2 WAT | 4416 | 23.525 | 29.907 | 2.579 | 1.00 40.00 |
| ATOM | 21347 | OH2 WAT | 4417 | 19.207 | .7.060 | -17.753 | 1.00 45.08 |
| | | | | | | | |
| MOTA | 21348 | OH2 WAT | 4418 | 27.504 | 25.535 | 33.468 | 1.00 36.75 |
| MOTA | 21349 | OH2 WAT | 4419 | 6.892 | -32.295 | 41.776 | 1.00 41.26 |
| MOTA | 21350 | OH2 WAT | 4420 | 17.067 | -1.474 | 58.088 | 1.00 34.61 |
| MOTA | 21351 | OH2 WAT | 4421 | 22.907 | 29.267 | 14.656 | 1.00 39.78 |
| MOTA | 21352 | OH2 WAT | 4422 | 6.224 | -49.951 | 10.824 | 1.00 28.84 |
| MOTA | 21353 | OH2 WAT | 4423 | -16.207 | 35.901 | 25.434 | 1.00 40.39 |
| ATOM | 21354 | OH2 WAT | 4424 | 0.738 | 15.078 | 67.744 | 1.00 35.60 |
| ATOM | 21355 | OH2 WAT | 4425 | -22.384 | 0.170 | 34.473 | 1.00 38.76 |
| MOTA | 21356 | OH2 WAT | 4426 | 52.264 | 32.015 | 13.016 | 1.00 52.37 |
| | | | | | -23.464 | | 1.00 32.37 |
| MOTA | 21357 | OH2 WAT | 4427 | 40.008 | 27.404 | 10.703 | 1.00 40.72 |

| MOTA | 21358 | OH2 W | АТ 4428 | 29.624 | 26.370 | 37.226 | 1.00 43.83 |
|--------------|----------------|--------|----------------|---------|-------------------|-----------------|--------------------------|
| ATOM | 21359 | OH2 WA | | | -33.128 | 69.819 | 1.00 36.99 |
| ATOM | 21360 | OH2 W | | 10.556 | 3.415 | 13.566 | 1.00 46.02 |
| | 21361 | OH2 W | | 8.523 | 41.333 | 58.843 | 1.00 39.73 |
| MOTA | 21362 | OH2 WA | | 33.167 | 23.763 | 37.373 | 1.00 28.85 |
| ATOM | | | | | | -17.090 | 1.00 47.32 |
| ATOM | 21363 | OH2 W | | | 2.684 | 36.535 | 1.00 37.32 |
| MOTA | 21364 | OH2 W | | -23.836 | | | 1.00 35.03 |
| MOTA | 21365 | OH2 W | | 19.214 | 12.147 | -5.475 | 1.00 33.97 |
| MOTA | 21366 | OH2 W | | 27.162 | -7.740 | 67.562 | |
| MOTA | 21367 | OH2 W | | -20.971 | -1.223 | 12.183 | 1.00 47.05 |
| MOTA | 21368 | OH2 W | | 19.674 | 12.470 | 63.556 | 1.00 44.37 |
| MOTA | 21369 | OH2 W | | -1.525 | 40.553 | 27.756 | 1.00 41.21 |
| MOTA | 21370 | OH2 W | | -18.654 | 1.585 | 28.426 | 1.00 32.42 |
| MOTA | 21371 | OH2 W | | 17.125 | 0.453 | 50.867 | 1.00 40.97 |
| MOTA | 21372 | OH2 W | | | -22.499 | -3.435 | 1.00 40.16 |
| MOTA | 21373 | OH2 W | | 14.381 | 25.984 | 34.791 | 1.00 37.01 |
| MOTA | 21374 | OH2 W | | | -17.781 | 2.660 | 1.00 35.38 |
| MOTA | 21375 | OH2 WA | | -34.581 | | 26.233 | 1.00 42.91 |
| MOTA | 21376 | OH2 W | | 24.684 | 23.141 | 0.831 | 1.00 35.73 |
| MOTA | 21377 | OH2 W | | 15.504 | 6.715 | 63.224 | 1.00 38.96 |
| MOTA | 21378 | OH2 W | | 19.904 | 21.033 | 71.538 | 1.00 43.76 |
| MOTA | 21379 | OH2 W | | -11.227 | 22.621 | -8.864 | 1.00 27.21 |
| MOTA | 21380 | OH2 W | | 22.345 | 0.986 | 14.851 | 1.00 34.11 |
| ATOM | 21381 | OH2 W | | -10.539 | | 27.450 | 1.00 36.84 |
| MOTA | 21382 | OH2 W | | 16.140 | 25.932 | 32.224 | 1.00 35.40 |
| ATOM | 21383 | OH2 W | | 44.961 | 30.241 | 15.396 | 1.00 37.99 |
| MOTA | 21384 | OH2 W | | | -25.015 | 12.520 | 1.00 36.11 |
| ATOM | 21385 | OH2 -W | AT 4455 | -20.127 | | 41.569 | 1.00 32.33 |
| MOTA | 21386 | OH2 W | AT 4456 | 5.429 | -56.224 | 24.411 | 1.00 42.80 |
| ATOM | 21387 | OH2 W | AT 4457 | 32.065 | 2.167 | 30.883 | 1.00 43.06 |
| MOTA | 21388 | OH2 W | AT 4458 | 5.091 | 42.861 | 7.752 | 1.00 39.50 |
| MOTA | 21389 | OH2 W | AT 4459 | -21.209 | -11.056 | 5.163 | 1.00 41.80 |
| ATOM | 21390 | OH2 W | AT 4460 | 19.803 | 9.836 | 20.265 | 1.00 40.87 |
| ATOM | 21391 | OH2 W | AT 4461 | 29.343 | 4.465 | 26.139 | 1.00 29.91 |
| MOTA | 21392 | OH2 W | AT 4462 | 10.788 | 42.451 | 0.401 | 1.00 42.38 |
| MOTA | 21393 | OH2 W | AT 4463 | -7.021 | -50.881 | 26.507 | 1.00 32.87 |
| MOTA | 21394 | OH2 W | AT 4464 | -19.249 | 19.648 | 45.938 | 1.00 29.54 |
| MOTA | 21395 | OH2 W | AT 4465 | 48.159 | 7.324 | 9.609 | 1.00 39.08 |
| MOTA | 21396 | OH2 W | AT 4466 | | -40.577 | 8.688 | 1.00 37.54 |
| ATOM | 21397 | OH2 W | | -25.910 | | 45.136 | 1.00 40.07 |
| MOTA | 21398 | OH2 W | | -22.226 | -2.802 | 33.260 | 1.00 35.07 |
| MOTA | 21399 | OH2 W | | -4.952 | 49.029 | 23.144 | 1.00 45.50 |
| MOTA | 21400 | OH2 W | | 17.417 | 13.858 | -4.051 | 1.00 38.03 |
| MOTA | 21401 | OH2 W | | 4.986 | | -15.614 | 1.00 30.12 |
| MOTA | 21402 | OH2 W | | | -22.524 | 1.908 | 1.00 36.21 |
| MOTA | 21403 | OH2 W | | | -47.999 | 29.175 | 1.00 23.74 |
| MOTA | 21404 | OH2 W | | -19.245 | 3.242 | 52.458 | 1.00 33.15 |
| MOTA | 21405 | OH2 W | | 41.831 | 21.851 | 70.956 | 1.00 36.15 |
| MOTA | 21406 | OH2 W | | | | -20.451 | 1.00 35.05 |
| MOTA | 21407 | OH2 W | | -23.878 | | -11.442 | 1.00 28.26 |
| MOTA | 21408 | OH2 W | | | -24.831 | 47.594 | 1.00 35.61 |
| MOTA | 21409 | OH2 W | | | 30.657 | | 1.00 47.25 |
| ATOM | 21410 | OH2 W | | 17.754 | 1.462 | 57.307 | 1.00 35.59 |
| MOTA | 21411 | OH2 W | | -7.414 | 21.345 | -1.587 | 1.00 30.73 |
| MOTA | 21412 | OH2 W | | 49.815 | 21.351 | 58.077 | 1.00 37.51 |
| MOTA | 21413 | OH2 W | | -15.491 | 44.459 | 7.923 | 1.00 50.41 |
| MOTA | 21414 | OH2 W | | | -22.551 | 5.047 | 1.00 36.58 |
| MOTA | 21415 | OH2 W | | | -12.564 | -0.579 | 1.00 37.00 |
| MOTA | 21416 | OH2 W | | | -13.615 | 27.066 | 1.00 19.93 |
| MOTA | 21417 | OH2 W | | -8.044 | 32.117 | 70.958 | 1.00 27.03 |
| ATOM | 21418 | OH2 W | | | -25.729 | 20.083 | 1.00 22.99 |
| MOTA | 21419 | OH2 W | | 17.072 | 17.442 | 39.782 | 1.00 27.80 |
| ATOM | 21420 | OH2 W | | | -43.716 | 22.448 | 1.00 25.25 |
| ATOM | 21421 | OH2 W | | 50.725 | -6.820 | 55.355 | 1.00 43.84 |
| ATOM | 21422 | OH2 W | | -19.456 | 26.078 -49.519 | 48.234 9.320 | 1.00 34.33 1.00 36.75 |
| ATOM | 21423 21424 | OH2 W | | | -49.519 | 2.269 | 1.00 36.75 |
| ATOM | 21424 | OH2 W | | | 36.702 | 49.212 | 1.00 34.78 |
| ATOM | | OH2 W | | 16.195 | | -20.690 | 1.00 32.39 |
| ATOM ATOM | 21426 21427 | OH2 W | | 26.413 | -5.902 | 59.650 | 1.00 48.10 |
| ATOM | 21427 | OH2 W | | -22.773 | 19.390 | 2.650 | 1.00 37.00 |
| | | OH2 W | | | -30.055 | 70.167 | 1.00 33.05 |
| ATOM | 21429 21430 | | | | 24.403 | -6.733 | 1.00 44.39 |
| ATOM ATOM | 21430 | OH2 W | | | -20.860 | 3.372 | 1.00 39.96 |
| ATOM | 21431 | OH2 W | | 3.145 | 16.448 | 33.272 | 1.00 42.41 |
| ATOM | 21432 | OH2 W | | | -30.786 | 61.572 | 1.00 30.34 |
| ATOM | 21434 | OH2 W | | 52.805 | 18.720 | 57.784 | 1.00 39.33 |
| | | | | | – - | | |

| ATOM | 21435 | OH2 WAT | 4505 | 31.760 | -29.715 | 16.803 | 1.00 42.71 |
|------|-------|---------|------|---------|---------|---------|------------|
| ATOM | 21436 | OH2 WAT | 4506 | 27.158 | -0.019 | -2.171 | 1.00 47.55 |
| MOTA | 21437 | OH2 WAT | 4507 | 16.391 | -6.880 | 13.945 | 1.00 27.93 |
| ATOM | 21438 | OH2 WAT | 4508 | -11.329 | 8.325 | 33.144 | 1.00 35.74 |
| | | | 4509 | | -18.654 | 31.647 | 1.00 41.23 |
| ATOM | 21439 | OH2 WAT | | | | | 1.00 35.82 |
| ATOM | 21440 | OH2 WAT | 4510 | 8.119 | 2.472 | 45.194 | |
| MOTA | 21441 | OH2 WAT | 4511 | | -26.276 | 1.441 | 1.00 43.41 |
| ATOM | 21442 | OH2 WAT | 4512 | 6.185 | 13.143 | 27.534 | 1.00 38.63 |
| ATOM | 21443 | OH2 WAT | 4513 | 15.834 | -35.849 | 46.381 | 1.00 39.03 |
| ATOM | 21444 | OH2 WAT | 4514 | 52.437 | 25.745 | 6.497 | 1.00 41.04 |
| ATOM | 21445 | OH2 WAT | 4515 | 5.343 | 4.118 | 14.468 | 1.00 33.27 |
| ATOM | 21446 | OH2 WAT | 4516 | 53.362 | 6.451 | 39.554 | 1.00 38.27 |
| ATOM | 21447 | OH2 WAT | 4517 | 1.590 | -4.443 | -22.357 | 1.00 33.22 |
| ATOM | 21448 | OH2 WAT | 4518 | 49.556 | -1.588 | 49.431 | 1.00 34.00 |
| ATOM | 21449 | OH2 WAT | 4519 | -28.945 | 3.556 | 61.373 | 1.00 43.53 |
| ATOM | 21450 | OH2 WAT | 4520 | -12.490 | 17.160 | 20.670 | 1.00 39.70 |
| ATOM | 21451 | OH2 WAT | 4521 | 40.918 | -3.831 | 38.596 | 1.00 26.45 |
| | 21452 | OH2 WAT | 4522 | 10.399 | -3.808 | 63.636 | 1.00 27.56 |
| ATOM | | | | | -42.115 | 6.281 | 1.00 43.08 |
| MOTA | 21453 | OH2 WAT | 4523 | | | | 1.00 45.08 |
| MOTA | 21454 | OH2 WAT | 4524 | -30.106 | -0.391 | 45.625 | |
| MOTA | 21455 | OH2 WAT | 4525 | 41.777 | | -15.445 | 1.00 37.86 |
| MOTA | 21456 | OH2 WAT | 4526 | 14.086 | 15.973 | 37.228 | 1.00 29.86 |
| MOTA | 21457 | OH2 WAT | 4527 | -22.519 | 27.041 | 47.602 | 1.00 45.34 |
| MOTA | 21458 | OH2 WAT | 4528 | -11.576 | 3.521 | -21.126 | 1.00 26.78 |
| ATOM | 21459 | OH2 WAT | 4529 | -2.842 | 24.071 | 13.955 | 1.00 37.20 |
| ATOM | 21460 | OH2 WAT | 4530 | 36.314 | -37.379 | 7.290 | 1.00 36.68 |
| MOTA | 21461 | OH2 WAT | 4531 | 8.937 | 41.604 | 63.559 | 1.00 44.67 |
| ATOM | 21462 | OH2 WAT | 4532 | | -15.555 | 37.510 | 1.00 35.99 |
| MOTA | 21463 | OH2 WAT | 4533 | | -30.744 | 64.478 | 1.00 33.23 |
| ATOM | 21464 | OH2 WAT | 4534 | 14.122 | 25.572 | 3.018 | 1.00 45.34 |
| ATOM | 21465 | OH2 WAT | 4535 | 29.990 | | -14.327 | 1.00 46.38 |
| | | OH2 WAT | 4536 | 17.429 | -9.357 | 65.683 | 1.00 44.69 |
| ATOM | 21466 | | | | | 74.869 | 1.00 34.09 |
| ATOM | 21467 | OH2 WAT | 4537 | | -17.310 | | |
| MOTA | 21468 | OH2 WAT | 4538 | 11.057 | 11.153 | 65.196 | 1.00 43.68 |
| ATOM | 21469 | OH2 WAT | 4539 | -13.688 | 21.726 | 22.028 | 1.00 48.02 |
| MOTA | 21470 | OH2 WAT | 4540 | -31.249 | -5.613 | 11.556 | 1.00 34.90 |
| ATOM | 21471 | OH2 WAT | 4541 | -7.066 | 28.532 | 37.518 | 1.00 37.48 |
| MOTA | 21472 | OH2 WAT | 4542 | 23.003 | 24.425 | 17.044 | 1.00 35.33 |
| MOTA | 21473 | OH2 WAT | 4543 | -3.469 | 27.584 | 73.860 | 1.00 39.05 |
| MOTA | 21474 | OH2 WAT | 4544 | 35.891 | 29.059 | 44.547 | 1.00 41.31 |
| ATOM | 21475 | OH2 WAT | 4545 | 18.800 | -1.059 | 10.975 | 1.00 15.84 |
| ATOM | 21476 | OH2 WAT | 4546 | -19.212 | -0.670 | 24.770 | 1.00 29.47 |
| ATOM | 21477 | OH2 WAT | 4547 | -16.028 | | -10.667 | 1.00 40.15 |
| ATOM | 21478 | OH2 WAT | 4548 | | -15.346 | 20.455 | 1.00 23.89 |
| | | OH2 WAT | 4549 | 42.287 | -4.979 | 41.504 | 1.00 27.98 |
| ATOM | 21479 | | | | | | 1.00 27.30 |
| MOTA | 21480 | OH2 WAT | 4550 | 38.305 | 9.987 | 71.347 | |
| ATOM | 21481 | OH2 WAT | 4551 | -11.381 | 38.933 | 24.989 | 1.00 49.32 |
| ATOM | 21482 | OH2 WAT | 4552 | -22.300 | 2.992 | 33.226 | 1.00 45.30 |
| MOTA | 21483 | OH2 WAT | 4553 | 6.931 | -6.229 | 41.554 | 1.00 41.06 |
| MOTA | 21484 | OH2 WAT | 4554 | 19.682 | -8.377 | 66.797 | 1.00 45.95 |
| MOTA | 21485 | OH2 WAT | 4555 | 36.306 | -36.168 | 62.243 | 1.00 35.31 |
| ATOM | 21486 | OH2 WAT | 4556 | 54.304 | 7.728 | 12.240 | 1.00 34.26 |
| MOTA | 21487 | OH2 WAT | 4557 | -28.537 | 7.332 | 49.621 | 1.00 40.13 |
| ATOM | 21488 | OH2 WAT | 4558 | 17.625 | 9.030 | 18.391 | 1.00 42.71 |
| ATOM | 21489 | OH2 WAT | 4559 | -12.739 | 20.162 | 7.607 | 1.00 32.46 |
| ATOM | 21490 | OH2 WAT | 4560 | -12.182 | 40.553 | 51.371 | 1.00 40.44 |
| ATOM | 21491 | OH2 WAT | 4561 | | -17.321 | 20.994 | 1.00 19.57 |
| ATOM | 21492 | OH2 WAT | 4562 | 9.509 | 14.689 | 21.947 | 1.00 18.00 |
| ATOM | 21493 | OH2 WAT | 4563 | 19.197 | 17.919 | 37.745 | 1.00 39.62 |
| ATOM | 21493 | OH2 WAT | 4564 | 8.296 | 41.620 | 10.968 | 1.00 40.32 |
| ATOM | 21494 | OH2 WAT | 4565 | 6.824 | | -17.793 | 1.00 45.81 |
| | | | 4566 | | -18.816 | 6.729 | 1.00 45.61 |
| MOTA | 21496 | OH2 WAT | | | | 54.082 | |
| MOTA | 21497 | OH2 WAT | 4567 | -12.020 | 40.602 | | 1.00 42.65 |
| ATOM | 21498 | OH2 WAT | 4568 | -15.024 | | -20.431 | 1.00 37.03 |
| ATOM | 21499 | OH2 WAT | 4569 | | -25.627 | -5.931 | 1.00 36.41 |
| ATOM | 21500 | OH2 WAT | 4570 | 11.961 | 16.248 | 26.219 | 1.00 31.42 |
| ATOM | 21501 | OH2 WAT | 4571 | 19.997 | 11.507 | 0.789 | 1.00 46.97 |
| MOTA | 21502 | OH2 WAT | 4572 | | -31.785 | 29.916 | 1.00 33.12 |
| MOTA | 21503 | OH2 WAT | 4573 | 30.687 | 11.177 | 59.321 | 1.00 35.02 |
| MOTA | 21504 | OH2 WAT | 4574 | -28.171 | 8.202 | -0.223 | 1.00 45.38 |
| ATOM | 21505 | OH2 WAT | 4575 | -23.907 | -0.946 | 0.147 | 1.00 47.86 |
| ATOM | 21506 | OH2 WAT | 4576 | 36.420 | -9.570 | -20.098 | 1.00 46.95 |
| MOTA | 21507 | OH2 WAT | 4577 | -9.302 | 25.934 | -13.864 | 1.00 17.87 |
| ATOM | 21508 | OH2 WAT | 4578 | | -31.859 | 17.185 | 1.00 41.07 |
| ATOM | 21509 | OH2 WAT | 4579 | 9.163 | 15.018 | 25.314 | 1.00 36.50 |
| ATOM | 21510 | OH2 WAT | 4580 | 20.941 | 19.630 | 26.829 | 1.00 35.95 |
| ATOM | 21511 | OH2 WAT | 4581 | 29.489 | -1.396 | -4.410 | 1.00 31.96 |
| | | J2 1171 | -501 | 27.407 | 1.570 | 1.110 | 54.50 |

| MOTA | 21512 | OH2 V | WAT 4582 | 33.238 | 34.672 | 55.740 | 1.00 46.22 |
|------|-------|-------|----------|---------|---------|---------|------------|
| MOTA | 21513 | OH2 V | WAT 4583 | -30.816 | -5.894 | 17.338 | 1.00 49.72 |
| ATOM | 21514 | OH2 V | WAT 4584 | | -28.094 | 76.769 | 1.00 34.85 |
| ATOM | 21515 | OH2 V | WAT 4585 | -2.179 | 15.453 | 30.418 | 1.00 40.59 |
| ATOM | 21516 | OH2 V | WAT 4586 | 4.279 | -17.186 | 76.947 | 1.00 48.31 |
| ATOM | 21517 | OH2 V | WAT 4587 | -0.036 | -14.038 | 25.792 | 1.00 21.21 |
| ATOM | 21518 | OH2 V | WAT 4588 | 29.067 | -1.678 | 2.086 | 1.00 24.42 |
| ATOM | 21519 | OH2 V | WAT 4589 | -5.344 | 11.926 | 31.843 | 1.00 29.45 |
| ATOM | 21520 | OH2 V | WAT 4590 | -3.000 | -4.011 | -20.507 | 1.00 33.38 |
| ATOM | 21521 | OH2 V | WAT 4591 | 16.416 | -34.157 | 13.726 | 1.00 32.70 |
| ATOM | 21522 | OH2 V | WAT 4592 | 42.496 | 30.507 | 62.292 | 1.00 31.93 |
| MOTA | 21523 | OH2 V | WAT 4593 | 45.544 | -3.876 | 0.068 | 1.00 37.84 |
| ATOM | 21524 | OH2 V | NAT 4594 | 4.284 | 25.647 | 44.152 | 1.00 46.08 |
| ATOM | 21525 | OH2 V | WAT 4595 | 28.936 | 0.551 | -17.645 | 1.00 49.26 |
| ATOM | 21526 | OH2 V | WAT 4596 | 28.309 | -1.764 | -7.219 | 1.00 34.20 |
| ATOM | 21527 | OH2 V | WAT 4597 | -0.139 | -4.683 | -4.704 | 1.00 40.66 |
| ATOM | 21528 | OH2 V | WAT 4598 | 38.002 | -39.295 | 28.778 | 1.00 37.91 |
| ATOM | 21529 | OH2 V | WAT 4599 | 1.896 | -10.498 | 26.814 | 1.00 40.28 |
| ATOM | 21530 | OH2 V | WAT 4600 | 10.875 | -31.201 | 46.215 | 1.00 46.59 |
| ATOM | 21531 | OH2 V | WAT 4601 | -17.789 | 11.593 | 42.545 | 1.00 40.33 |
| ATOM | 21532 | OH2 V | WAT 4602 | 13.281 | -34.722 | 45.502 | 1.00 43.03 |
| MOTA | 21533 | OH2 V | WAT 4603 | 15.546 | 2.812 | 48.750 | 1.00 34.98 |
| MOTA | 21534 | OH2 V | WAT 4604 | -24.408 | -0.962 | 68.815 | 1.00 34.14 |
| ATOM | 21535 | OH2 V | WAT 4605 | 27.530 | 8.533 | -3.110 | 1.00 46.99 |
| MOTA | 21536 | OH2 V | WAT 4606 | -5.207 | -2.672 | -4.358 | 1.00 37.50 |
| MOTA | 21537 | OH2 V | NAT 4607 | -6.846 | -4.949 | 54.526 | 1.00 33.19 |
| ATOM | 21538 | OH2 V | WAT 4608 | -8.773 | -28.684 | 66.448 | 1.00 41.34 |
| MOTA | 21539 | OH2 V | WAT 4609 | 15.694 | -33.293 | 11.109 | 1.00 42.89 |
| ATOM | 21540 | OH2 V | WAT 4610 | 25.189 | 7.699 | -4.734 | 1.00 38.08 |
| ATOM | 21541 | OH2 V | WAT 4611 | -25.724 | -20.312 | 42.518 | 1.00 44.59 |
| ATOM | 21542 | OH2 V | WAT 4612 | 30.872 | -53.539 | 20.326 | 1.00 48.78 |
| ATOM | 21543 | OH2 V | WAT 4613 | 7.005 | -17.629 | 0.602 | 1.00 47.16 |
| ATOM | 21544 | OH2 V | WAT 4614 | -20.076 | 21.041 | 2.976 | 1.00 50.56 |
| ATOM | 21545 | OH2 V | WAT 4615 | 49.790 | 17.372 | -5.207 | 1.00 53.06 |
| ATOM | 21546 | OH2 V | WAT 4616 | 45.033 | 0.193 | 5.524 | 1.00 36.67 |
| ATOM | 21547 | OH2 V | WAT 4617 | 3.384 | 12.364 | 26.877 | 1.00 47.24 |
| MOTA | 21548 | OH2 V | WAT 4618 | -23.460 | -11.122 | 39.780 | 1.00 36.40 |
| MOTA | 21549 | OH2 V | WAT 4619 | 36.510 | -18.235 | -14.040 | 1.00 44.41 |
| MOTA | 21550 | OH2 V | WAT 4620 | 27.674 | 11.270 | 60.667 | 1.00 36.19 |
| MOTA | 21551 | OH2 V | WAT 4621 | -25.671 | -31.027 | 5.734 | 1.00 35.54 |
| ATOM | 21552 | OH2 V | WAT 4622 | -33.918 | -10.844 | 11.974 | 1.00 43.33 |
| END | | | | | | | |

Table 2 Crystallographic data quality, phasing, refinement and model quality

| Space group & Cell parameters (Å) | $P2_1 \ a = 87.8$ | $P2_1 \ a = 87.8 \ b = 155.4 \ c = 209.9 \ \beta = 99.3^{\circ}$ | 30 | $P2_1 \ a = 86.1 \ b = 157.2 \ c = 100.2 \ \beta = 97.4^{\circ}$ |
|--|----------------------------|--|---------------|--|
| Data quality | . , | | | |
| Data set | Edge | Peak | Remote | Native |
| Wavelength (Å) | 0.97939 | 0.97927 | 0.9393 | 0.979 |
| Limiting resolution (Å) | 3.1 | 2.8 | 2.8 | 1.8 |
| Races | 0.161 | 0.120 | 0.131 | 0.103 |
| < I/al > (high resolution) | 12.8 (2.6) | 25.6 (6.0) | 13.3 (3.3) | 15.9 (2.1) |
| Completeness | 0.994 | 0.999 | 1.0 | 0.94 |
| No. unique restexions (multiplicity) | 100 734 (3.5) | 136 609 (10.6) | 136 664 (3.3) | 229 086 (4.5) |
| Experimental f / f' (electrons) ^b | -9.9 / 2.9 | -8.6 / 5.4 | -1.3 / 3.2 | |
| Refinement (40 - 1.7 Å) | | | | |
| Reyse | 0.229 (highest resolution: | resolution: 0.286) | | |
| Rined | 0.263 (| 0.318) | | |
| No. reflexions: working / test ^d | 206 168 / 22 908 | 80 | | |
| No. atoms (residues) | 19 820 (2 640) | | | |
| . No. waters | 1 610 | | | |
| Model quality | | | | |
| Ramachandran plot: % residues favourable | 90.4 | | | |
| % unfavourable | None | | | |
| R.m.s. deviations: Bond lengths | 0.006 | | , | |
| Bond angles | 1.2 | | | |
| Dihedral angles | 22.1 | | | |

 $^{\text{\tiny R}}R_{\text{\tiny R}\text{\tiny R}\text{\tiny B}} = \left[\Sigma_{\text{\tiny h}} w \Sigma_{i} | c_{\text{\tiny h}} > l_{\text{\tiny h},i} \right] / \Sigma_{\text{\tiny L},i} l_{\text{\tiny h},i} \text{ where } w = \sqrt{\left[l_{\text{\tiny h}} (n_{\text{\tiny h}} - 1) \right]} \text{ and } c_{\text{\tiny h}} > = \left[\Sigma_{i}^{\text{\tiny I}} l_{\text{\tiny h},i} \text{ the multiplicity-weighted } R_{\text{\tiny $yymm$}} \left[\text{Diederichs, } 1997 \# 155 \right]$

 $^dR_{\rm fre}$: cross-validation $R_{
m cryst}$, i.e. calculated using randomly selected test data not used in refinement.

 $^cR_{ctys} = \Sigma ||F_0| - |F_c||\Sigma |F_0|$; F_0 and F_c are observed and calculated structure factor amplitudes.

^b Estimates from CHOOCH (Evans, 1999)